WATER DEUTERIUM FRACTIONATION IN THE INNER REGIONS OF TWO SOLAR-TYPE PROTOSTARS

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ABSTRACT

The [HDO]/[H2O] ratio is a crucial parameter for probing the history of water formation. So far, it has been measured for only three solar-type protostars and yielded different results, possibly pointing to a substantially different history in their formation. In the present work, we report new interferometric observations of the HDO 4_2,2–4_2,3 line for two solar-type protostars, IRAS2A and IRAS4A, located in the NGC 1333 region. In both sources, the detected HDO emission originates from a central compact unresolved region. A comparison with previously published interferometric observations of the H218O 3_1,3–2_2,0 line shows that the HDO and H2O lines mostly come from the same region. A non-LTE large velocity gradient analysis of the HDO and H218O line emissions, combined with published observations, provides an [HDO]/[H2O] ratio of 0.3%–8% in IRAS2A and 0.5%–3% in IRAS4A. First, the water fractionation is lower than that of other molecules such as formaldehyde and methanol in the same sources. Second, it is similar to that measured in the solar-type protostar prototype, IRAS16293-2422, and, surprisingly enough, larger than that measured in NGC 1333 IRAS4B. The comparison of the measured values toward IRAS2A and IRAS4A with the predictions of our gas–grain model GRAINOBLE gives similar conclusions to those for IRAS 16293, arguing that these protostars share a similar chemical history, although they are located in different clouds.

Key words: astrochemistry – ISM: abundances – ISM: individual objects (NGC 1333-IRAS2A, NGC 1333-IRAS4A) – ISM: molecules – stars: formation

1. INTRODUCTION

The formation of solar-type protostars is triggered by the gravitational collapse of dense fragments of molecular clouds, the so-called prestellar cores. In molecular clouds and prestellar cores, the low temperature and interstellar UV flux promote the formation of icy mantles around the dust grains. These mantles are mainly composed of H2O, CO, CO2, H2CO, or CH3OH (see Boogert & Ehrenfreund 2004). The last two become abundant with the freezeout of CO. In addition, the CO freeze-out coupled with the cold conditions enhances the abundance of the deuterated molecules (see Ceccarelli et al. 2007; Caselli et al. 2008).

Several theoretical studies have shown that the molecular deuteration is very sensitive to the physical conditions. For instance, the deuteration of gaseous species increases with the total density nH and decreases with the temperature (see Millar et al. 1989; Roberts et al. 2003). Similarly, the deuteration of icy species formed on the grain surfaces by H and D atom addition reactions, such as H2O, H2CO, and CH3OH, depends on the gaseous atomic [D]/[H] ratio, which also increases with the density and the CO freezeout at low temperatures (Cazaux et al. 2011; Taquet et al. 2012b, 2013).

In theory, therefore, the deuteration of different mantle species can be used to reconstruct the history of the ice formation and, consequently, of the protostar (e.g., Taquet et al. 2013). In practice, unfortunately, the direct measurement of the deuteration of frozen species is not possible. Observations of solid HDO toward protostars only yielded upper limits (with HDO/H2O ≲ few percent; Dartois et al. 2003; Parise et al. 2003). However, one can observe these species where the icy mantles sublimate, for example, in the hot corino regions. Since the timescale needed to significantly alter the deuteration after the ice sublimation is longer than the typical age of Class 0 protostars (∼103 versus ∼104 yr; Charnley et al. 1997; André et al. 2000), the measured deuteration of the gaseous mantle species likely reflects that in the ices prior to the sublimation. A comparison between the measured and predicted deuteration in interstellar ices is, therefore, possible.

In Taquet et al. (2013), we did a first study by comparing the predictions of our gas–grain GRAINOBLE model (Taquet et al. 2012a) with the observations toward the protostar IRAS16293-2422 (hereafter IRAS16293). This source displays a very high deuterium fractionation of formaldehyde and methanol (with D/H ratios of 15% and 40%, respectively; see Loinard et al. 2001; Parise et al. 2002, 2004) and a lower fractionation of water (0.1%–3%; see Butner et al. 2007; Vastel et al. 2010; Coutens et al. 2012, 2013; Persson et al. 2013). We concluded that the lower fractionation of water with respect to that of formaldehyde and methanol is likely due to a different epoch of formation of the three species. Water is predicted to be mainly produced during the molecular cloud phase, while most of formaldehyde and methanol are formed during the colder and denser prestellar phase. We carried out a similar study using the measured deuteration of H2O, H2CO, and CH3OH toward the outflow shock L1157-B1 and concluded that this site had a similar sequence for the formation of the ice, but in a less dense environment (Codella et al. 2012).

Encouraged by these two studies, here we extend the analysis to other solar-type protostars with the goal of reconstructing the formation history of their ices and compare it with the two previous cases. Ultimately, a similar study in a large sample of solar-type protostars will provide us with a more complete...
picture of how the environment influences the chemical composition of the ices and will supply strong constraints to the theory.

Although the fractionation of formaldehyde and methanol has been measured toward several solar-type protostars (Parise et al. 2002, 2004, 2005, 2006), observational studies of deuterated water are scarce. In NGC 1333-IRAS4B, the non-detection of the HDO line at 225.6 GHz yields an upper limit to the [HDO]/[H₂O] ratio of <6 × 10⁻⁴ (Jørgensen & van Dishoeck 2010). In NGC 1333-IRAS2A, several HDO and H₂O lines have been observed with single-dish telescopes. Using the Herschel Space Observatory, Kristensen et al. (2010) observed a broad outflow component for several H₂O lines, but could not accurately estimate the water abundance in the warm compact region. In contrast, Liu et al. (2011) derived the HDO abundance profile in the warm and cold regions of the envelope. However, single-dish telescopes also encompass the cold envelope and the possible outflow component. Complementary interferometric observations, with arcsecond resolutions, are needed to resolve the emission coming from the hot corinos, where the ices are sublimated and the deuteration likely reflects the ice pristine deuteration (Jørgensen & van Dishoeck 2010; Persson et al. 2013).

In this Letter, we present interferometric IRAM Plateau de Bure observations of the HDO 4₂₂–4₂₃ line at 143 GHz toward NGC 1333-IRAS2A (hereinafter IRAS2A) and NGC 1333-IRAS4A (hereinafter IRAS4A). These sources are located in the Perseus complex, in the NGC 1333 cloud, whose distance is about 220 pc (Cernis 1990). They were selected because they are the two line brightest low-mass protostars after IRAS16293 due to their distance and their luminosity and because interferometric observations of H₂²O have been recently obtained by Persson et al. (2012) toward them. The [HDO]/[H₂O] ratio derived in the present work, combined with previous observations of deuterated formaldehyde and methanol, will be compared with the predictions of our gas–grain model GRAINOBLE (Taquet et al. 2013) to reconstruct the chemical history of these two protostars.

2. OBSERVATIONS AND RESULTS

The two low-mass Class 0 protostars IRAS2A and IRAS4A were observed with the IRAM Plateau de Bure Interferometer on 2010 August 1, August 3, and 2011 March 10 and in the C and D configurations of the array. Due to the proximity to each other, the two sources were observed in the same track. The 4₂₂–4₂₃ HDO transition at 143.727 GHz and the 2 mm continuum emission have been obtained simultaneously using the WIDEX correlator, with a 1.8 GHz bandwidth centered at 143.5 GHz, and providing a spectral resolution of 1.95 MHz (4 km s⁻¹). Phase and amplitude were calibrated by performing regular observations of the nearby point sources 3C454.3, 3C84, and 0333+321. The amplitude calibration uncertainty is estimated to be ~20%.

The data calibration and imaging were performed using the CLIC and MAPPING packages of the GILDAS software.⁵ Continuum images were produced by averaging line-free channels in the WIDEX correlator before the Fourier transformation of the data. The coordinates of the sources and the size of the synthesized beams are reported in Table 1.

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³ The GILDAS package is available at http://www.iram.fr/IRAMFR/GILDAS.
central regions. The fluxes are given in Table 2 and are used in the next section to estimate the $[\text{HDO}]/[\text{H}_2\text{O}]$ ratio.

3. DEUTERIUM FRACTIONATION OF WATER

3.1. Method

A single transition line of HDO and $\text{H}^{18}\text{O}$ does not allow us to derive an accurate estimate of the HDO and $\text{H}_2\text{O}$ column densities toward the two protostars and, therefore, of $[\text{HDO}]/[\text{H}_2\text{O}]$. In order to derive the physical conditions of the line emitting gas and the relevant column densities, we compared the predictions from a non-LTE large velocity gradient (LVG) code (Ceccarelli et al. 2003) with our observations and the observations by Liu et al. (2011) of several HDO lines toward $\text{IRAS2A}$, obtained with the IRAM 30 m, JCMT, and APEX telescopes. We considered the collisional coefficients from Daniel et al. (2011) for $\text{H}^{18}\text{O}$ and from Faure et al. (2012) for HDO. The Einstein coefficients are from the Jet Propulsion Laboratory molecular database (Pickett et al. 1998).

We ran a grid of models covering a large parameter space in kinetic temperature $T_{\text{kin}}$ (15 values from 70 to 220 K), $n_{\text{H}}$ (15 values from $1 \times 10^6$ to $1 \times 10^9$ cm$^{-3}$), HDO column density $N(\text{HDO})$ (15 values from $8 \times 10^{14}$ to $1 \times 10^{17}$ cm$^{-2}$), and source size $\theta_s$ (30 values from 0.1 to 200 arcsec). In addition, we considered three values for the ortho-to-para ratio (opr) of $\text{H}_2$: 10$^{-3}$ (namely, all $\text{H}_2$ molecules are in the para state), 1, and 3 (thermal equilibrium value at $T > 50$ K). To find the best fit to the data, we excluded the 464 GHz line observed by Liu...
et al. (2011) as it may be contaminated by the cold envelope emission, given its low energy level (22 K).

### 3.2. Results

**IRAS2A.** We ran the grid of models to reproduce the emission of the HDO lines toward IRAS2A. The H$_2$ op has a low influence on the column densities derived from the observations. Varying the H$_2$ op between 0.1 and 3 causes a small variation of the results, by no more than 20%, namely, within the uncertainties of the observations. In the following, we consider an H$_2$ op of 3. The flux of all the HDO lines are well reproduced (reduced $\chi^2 < 1$) for $T_{\text{kin}} \sim 75$–80 K, $\theta_s = 0'4$, and a wide range of $n_\text{H}_2$ between 6 × 10$^5$ and 2 × 10$^8$ cm$^{-3}$. The derived $N$(HDO) varies between 5 × 10$^{17}$ and 10$^{19}$ cm$^{-2}$ and decreases with $\theta_s$. To evaluate the H$_2$O column density $N$(H$_2$O) from the 203.4 GHz transition, we considered three physical cases that reproduce the emission of the HDO lines (see Table 3). The density used in Case 1 (6 × 10$^5$ cm$^{-3}$) is similar to the density used by Maret et al. (2004) for reproducing the H$_2$CO emission with a non-LTE LVG analysis. The densities used in Cases 2 and 3 are slightly lower than the density in the hot corino region (where the temperature is higher than 100 K) of IRAS2A derived by Jørgensen et al. (2002). Higher densities do not reproduce the observed HDO emission (the reduced $\chi^2$ increases to values much higher than 1). Regardless of the density, the derived column density of H$_2$O is equal to (6–7) × 10$^{16}$ cm$^{-2}$. Note that at $n_\text{H}_2 = 6 × 10^8$ cm$^{-3}$, the line weakly masers (see also Neufeld & Melnick 1991). The column densities we obtain are slightly higher, by a factor of two, than that derived by Persson et al. (2012). The difference can, therefore, come from a combination of the LTE versus non-LTE population, gas temperature, and line opacity (in our model, it is 1.4). The low temperature could indicate that the gas is thermally decoupled from the dust. $N$(H$_2$O) can then be derived by assuming an isotopic abundance ratio $^{16}$O/$^{18}$O of 560 (Wilson & Rood 1994) and an op of 3 (see Emprechtinger et al. 2010; 2013). Depending on $n_\text{H}_2$, we derive an [HDO]/[H$_2$O] abundance ratio between 0.3% and 8% (see Table 3).

**IRAS4A.** For IRAS4A, no other HDO lines but the line observed in this work are available. The flux of the HDO and H$_2$O lines is, therefore, compared with the predictions obtained by using the same set of physical conditions as for IRAS2A. We also used another set of parameters presenting a larger source size $\theta_s$ of 0'8, consistent with the upper limit

given by Persson et al. (2012) for the H$_2$O transition. The increase in $\theta_s$ slightly decreases the column density of HDO and H$_2$O by approximately the same factor (2–3), giving similar results to those by Persson et al. (2012). The [HDO]/[H$_2$O] ratio, therefore, decreases by a factor of two, at maximum. For both sets of physical conditions, we predict an [HDO]/[H$_2$O] abundance ratio between 0.5% and 3% (see Table 3).

### 4. DISCUSSION AND CONCLUSIONS

The first result of this work is the relatively high water deuterium, ∼1%, in IRAS2A and IRAS4A. In IRAS2A, this value is compatible with the lower limit derived by Liu et al. (2011) in the same source (see Section 1). In IRAS4A, this is the first published estimate.
Second, as in IRAS16293 and L1157-B1, the water deuteration is lower, by about one order of magnitude, than the deuteration of formaldehyde and methanol in the same sources, previously measured by Parise et al. (2006).

Third, the water deuteration in IRAS2A and IRAS4A is very similar to that measured in IRAS16293 by Coutens et al. (2012), ~3%, but higher than the ratio derived by Persson et al. (2013) in the same source. The difference between the two results might come from the choice of the method. Persson et al. (2013) derived the [HDO]/[H2O] ratio from few lines by assuming LTE population and optically thin emission, whereas the quoted column density implies a line opacity ~5 and the 203 GHz line may maser (see above). On the contrary, Coutens et al. (2012) uses single-dish observations which also encompass the cold envelope even though most of the lines have $E_{ap} > 50$ K, so that the contamination from the outer cold envelope is accounted for.

The ratio is at least one order of magnitude larger than the value measured in IRAS4B, $<6 \times 10^{-3}$, by Jørgensen & van Dishoeck (2010), despite the fact that this source lies in the same molecular cloud, NGC 1333, as IRAS2A and IRAS4A and it is only ~15″ away from IRAS4A (Sandell et al. 1991). To add to this oddity, the deuteration of formaldehyde and methanol in IRAS4B is very similar to that measured in IRAS2A and IRAS4.

Figure 2 summarizes the situation with a plot of the measured deuteration of water, formaldehyde, and methanol in the outflow shock L1157-B1 and in the protostars IRAS 16293, IRAS2A, IRAS4A, and IRAS4B. In the same figure, we also show the theoretical predictions by the gas–grain model GRAINOBLE (Taquet et al. 2013). Briefly, the model follows the multilayer formation of deuterated ices with a pseudo time-dependent approach. We report the icy [HDO]/[H2O] ratio computed at $3 \times 10^3$ yr (the typical age of prestellar cores) for different constant densities and temperatures, $n_v = 10$ mag. The H$_2$ opr, which is difficult to constrain observationally, is one of the key parameters in setting the [HDO]/[H2O] ratio (Taquet et al. 2013). Following the value derived by Dislaire et al. (2012) toward IRAS 16293, we used a H$_2$ opr of $10^{-3}$.

The comparison between the observations and the theoretical predictions shows that the [HDO]/[H2O] ratio measured in IRAS2A and IRAS4A is reproduced for a large range of physical conditions: $n_H \sim 10^3$–$10^4$ cm$^{-3}$ for $T = 10$ K and $n_H \sim 10^3$–$10^4$ cm$^{-3}$ for $T = 20$ K. On the contrary, our model cannot reproduce the [HDO]/[H2O] value reported by Jørgensen & van Dishoeck (2010) for densities larger than $10^5$ cm$^{-3}$. One possible explanation is that water ice has formed at a lower H$_2$ opr (see Taquet et al. 2013) or the model is missing some ingredients regarding the deuterated ice formation.

As in our previous work, we note that the larger deuteration of formaldehyde and methanol testifies to a formation of these species on the grain surfaces at a later and higher density stage than water, likely the prestellar core phase.

Finally, NGC 1333 is a very active star-forming region undergoing the destruction and alteration from various outflows of the first-generation stars that might have initiated the formation of IRAS2A and IRAS4A (Liseau et al. 1988; Warin et al. 1996; Lefloch et al. 1998; Knee & Sandell 2000), whereas the cloud containing IRAS16293 is relatively quiescent (Mizuno et al. 1990). Nevertheless, the similar deuterium fractionation derived in IRAS2A, IRAS4A, and IRAS 16293 suggests that these protostars have followed a similar chemical history even though they are located in very different environments. However, the [HDO]/[H2O] ratio observed in IRAS4B by Jørgensen & van Dishoeck (2010) and in IRAS 16293 by Persson et al. (2013) does not fit with this conclusion and remains puzzling.

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REFERENCES

Andr´e, P., Ward-Thompson, D., & Barsony, M. 2000, in Protostars and Planets IV, ed. V. Mannings, A. P. Boss, & S. S. Russell (Tucson, AZ: Univ. Arizona Press), 59

Boogert, A. C. A., & Ehrenfreund, P. 2004, in ASP Conf. Ser. 309, The Astrophysics of Dust, ed. A. N. Witt, G. C. Clayton, & B. T. Draine (San Francisco, CA: ASP), 547

Butner, H. M., Charnley, S. B., Ceccarelli, C., et al. 2007, ApJL, 659, L137

Caselli, P., Vastel, C., Ceccarelli, C., et al. 2008, A&A, 492, 703

Cazaux, S., Caselli, P., & Spaans, M. 2011, ApJL, 741, L34

Ceccarelli, C., Caselli, P., Herbst, E., Tielens, A. G. G. M., & Caux, E. 2007, in Protostars and Planets V, ed. B. Reipurth, D. Jewitt, & K. Keil (Tucson, AZ: Univ. Arizona Press), 47
