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DEUTERIUM ENHANCEMENT IN WATER TOWARD ORION IRc2 DEDUCED FROM HDO LINES ABOVE 800 GHz

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ABSTRACT

We present the first detection of two submillimeter lines of HDO in the KL region of Orion: $J_{Ka,Kb} = 2_{1,2} \rightarrow 1_{1,1}$ (848.9619 GHz), and $1_{1,1} \rightarrow 0_{0,0}$ (893.6387 GHz). The first line has been mapped at 10″ angular resolution. These transitions involve some of the lowest energy levels of HDO and have the shortest wavelengths accessible from the ground. Therefore, they provide a perfect tool to complement previous works that made use of millimeter HDO transitions involving similar energy levels ($1_{1,0} \rightarrow 1_{1,1}$ at 80.6 GHz, $2_{1,1} \rightarrow 2_{1,2}$ at 241.6 GHz, and others). The two submillimeter lines arise from the moderate expanding material or "Plateau" ($v_{LSR} \sim 9$ km s^{-1}, $\Delta v \geq 20$ km s^{-1}). The emission is very compact in both HDO transitions (no more extended than ∼40″–45″) with similar intensities, line shapes, and line widths. The Hot Core seems completely hidden in our data in contrast with the majority of other millimeter-wave observations. This fact can only be explained if the Hot Core is embedded or behind the region of the outflow. The high line opacity of the submillimeter HDO lines would then hide the Hot Core emission. A comparison with our previously published high angular resolution para-H_2O data ($3_{1,3} \rightarrow 2_{2,0}$ at 183.31 GHz, and $5_{1,5} \rightarrow 4_{2,2}$ at 325.15 GHz) can be performed to derive the HDO/H_2O ratio in the "Plateau" warm molecular environment. We have found this ratio to be in the range 0.004 to 0.01. Such a high value, taking into account that the kinetic temperature exceeds 150 K, clearly supports the idea that the observed HDO has recently evaporated from dust grain mantles.

Subject headings: ISM: abundances — ISM: individual (Orion IRc2) — line: profiles — radio lines: ISM — submillimeter

1. INTRODUCTION

Although many lines of water vapor have been detected since its early discovery in space by Cheung et al. (1969) and despite the fact that it is probably one of the most abundant molecules in warm interstellar clouds, the strong observational constraints affecting its study have hidden most of the information from our sight until very recently. In the past decade the possibility of detecting from the ground some millimeter (Cernicharo et al. 1990) and submillimeter (Menten, Melnick, & Phillips 1990a; Menten et al. 1990b) transitions of H_2O was demonstrated and some important studies were conducted (González-Alfonso et al. 1996; Cernicharo et al. 1994, 1999, hereafter Cer94 and Cer99). However, almost certainly all the observed $H_2^{16}O$ transitions were masing to some degree. To avoid this problem, and thanks in part to the development of submillimeter-wave technology, lines involving the lowest energy levels of isotopic species of water vapor have been used for ground-based and airborne observations (Jacq et al. 1990; Zmuidzinas et al. 1995). Finally, in the past 3 or 4 years direct observations of transitions involving the lowest levels of ortho- and para-H_2O have been performed due to the availability of space-borne telescopes: *ISO* and *SWAS*. Many of these studies (e.g., Harwit et al. 1998; González-Alfonso et al. 1998; van Dishoeck et al. 1998; Cer99; Melnick et al. 2000) have been devoted to the region surrounding Orion IRc2, because it is the closest site possessing the physical conditions needed for strong water emission. However, the main drawbacks to these data are, in general, low angular resolution, high opacity of the observed lines, poor spectral resolution (for space-borne observations), and the masing nature of the lines (for those observed with ground-based instruments). However, Cer94 and Cer99 have used adequate radiative transfer codes that allow an estimation of H_2O abundances in Orion and other sources from the 183 and 325 GHz lines.

In order to access HDO thermal emission and to obtain much better angular and spectral resolution we have selected two consecutive transitions of HDO connecting three of the lowest energy levels ($2_{1,2}$, $1_{1,1}$, and $0_{0,0}$, see Fig. 1) at frequencies above 800 GHz, that are reachable from the ground at high and dry observatories such as the Caltech Submillimeter Observatory (CSO) on the Mauna Kea summit.

The HDO data presented here are a step forward in our high-resolution study aimed at deriving water vapor abundance and physical conditions in the environment of Orion IRc2. In addition, the data allow a fresh look at the D/H enrichment in Orion relative to the interstellar medium, pointed out shortly after HDO was first discovered at millimeter wavelengths in this source by Turner et al. (1975). Studies of this enrichment include Beckman et al. (1982), Olofsson (1984), Moore, Huguenin, & Langer (1986), Plambeck & Wright (1987), and Jacq et al. (1990). Other deuterated species were studied for example by Walmsley et al. (1987) and Charnley, Tielens, & Rodgers (1997). The $H_2^{16}O$ data used for the comparison involve the 183 and 325 GHz lines (Cer94; Cer99) at similar angular resolutions.

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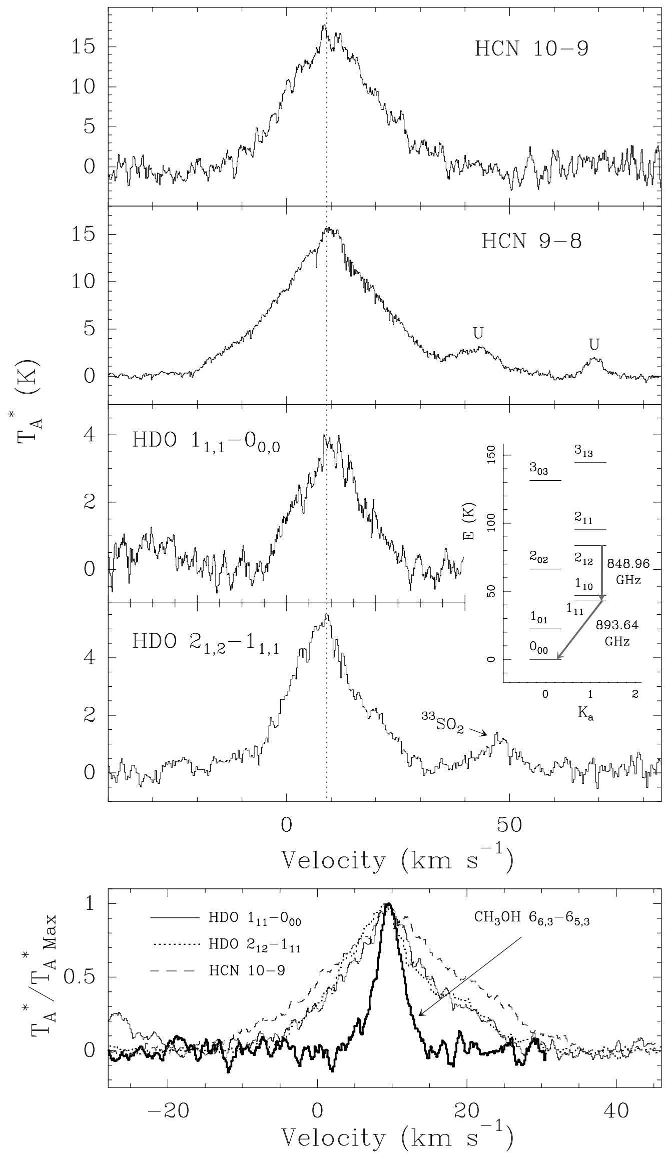

FIG. 1.—Strongest HDO and HCN spectra detected toward Orion IRc2 in this work. The average of these lines over the nine central, strongest positions, normalized to their peak intensity are compared to the same average on the methanol 890.450 GHz line to stress the line width difference of the studied transitions of HDO and HCN respect to a typical Hot Core line (CH_3OH).

2. OBSERVATIONS AND RESULTS

2.1. *Observations*

The observations were performed with the 10.4 m telescope of the Caltech Submillimeter Observatory at the summit of Mauna Kea (Hawaii) during four different runs in 2000 January, March, and October and 2001 February. The receiver is a helium-cooled SIS mixer operating in double-sideband mode (DSB) designed to fully cover the 780–910 GHz atmospheric window (see Kooi et al. 2000).

The sideband origin of the lines was checked by slightly changing the frequency (a few tens of MHz) and repeating the observation. In addition to the HDO lines we detected CH_3OH $6_{6,3}$–$6_{5,3}$ (at 890.450 GHz), a line that originates in the Hot Core, and $^{33}SO_2$ (at 848.8693 GHz). The central position was also observed in HCN 9–8 (797.4337 GHz) and we performed a map in HCN 10–9 (885.9708 GHz). The back end consisted of a 1024 channel acousto-optic spectrometer covering a bandwidth of 500 MHz, thus providing a velocity resolution of $\Delta v = 0.1723$ km s^{-1} at 850 GHz.

The Orion-IRc2 maps were carried out using the chopping secondary method at a frequency of 1.123 Hz and a step of 120″ in azimuth (that proved to be enough once we performed a previous check of the extension of the emission by means of several position-switched scans at different separations on the sky).

2.2. *Relative Pointing and Calibration*

Since the observations above 790 GHz presented in this paper began shortly after the receiver was installed for the first time at the telescope, and they took several observing runs to complete with different weather conditions, special care was taken for the pointing, focus, and relative calibration. The data had a reasonable pointing consistency (∼4″) with earlier CSO maps performed around 325 GHz (Cer99). In some cases, lines simultaneously present in the back end and known to arise almost exclusively from the Hot Core, such as CH_3OH $6_{6,3}$–$6_{5,3}$, were used to relocate the observation or the whole map of our target line.

The best atmospheric conditions occurred on 2000 January 24, when the HDO $2_{1,2} \rightarrow 1_{1,1}$ map presented here was achieved. We reached system temperatures as low as 1700 K at 849 GHz. Using those data and the multilayer atmospheric radiative transfer model ATM (Cernicharo 1985, 1988; Pardo, Cernicharo, & Serabyn 2001) the opacities predicted at the working frequencies were in very good agreement with the ones obtained from the sky dips (within 5%). All these facts make us very confident about the calibration of the data. The T_a^* output obtained from the "chopper-calibration" method (Penzias & Burrus 1973) was corrected to account for the fact that only one calibration load is used (Pardo et al. 2002, in preparation). The beam efficiency of the telescope measured at 807 GHz was 27% using Mars (measured HPBW at that frequency: 11″.5).

2.3. *Results*

The line profiles of the two observed HDO transitions are very similar at the positions of their respective maximum emission and present basically the same intensity within the calibration uncertainty. They extend from about −10 to ∼35 km s^{-1} with a peak at ∼9 km s^{-1}. These are the characteristics of the emission arising from the moderate velocity "Plateau" material. Further evidence of the Plateau origin of our observed HDO lines comes from comparing them with the HCN 9–8 and 10–9 lines (Plateau) and the CH_3OH $6_{6,3}$–$6_{5,3}$ line (Hot Core), also observed during this study (Fig. 1).

The extension of the HDO $2_{1,2}$–$1_{1,1}$ (Fig. 2) and $1_{1,1}$–$0_{0,0}$ (map not shown here) emission is small (HPW ∼15″) with no detection beyond 35″–40″ from the IRc2 position. Therefore, HDO does not trace the extended emission observed at 183 GHz in H_2O (Cer94). HCN 10–9, although just a bit more extended, is not seen beyond 1′ from IRc2. The compactness of the HDO emission confirms earlier results from observations of HDO millimeter lines which show different components, including the Plateau, depending on the transition: Olofsson (1984) and Plambeck & Wright (1987) (emission region smaller than 25″ at 80.6 GHz), Moore et al. (1986) and Jacq et al. (1990) (emission region 10″–15″ in size at 241 GHz). However, there is a fundamental difference between our results and the cited previous HDO millimeter

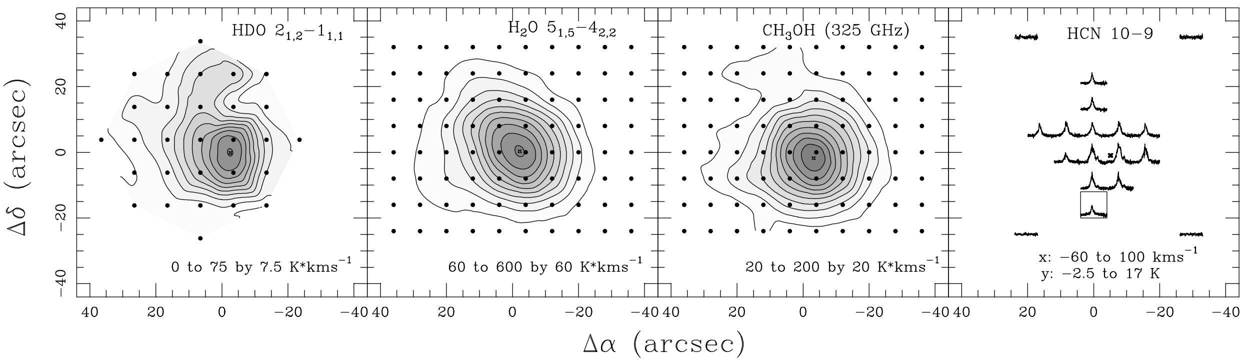

FIG. 2.—Maps of HDO $2_{1,2}$–$1_{1,1}$ and HCN 10–9 obtained toward Orion IRc2 (T_A^* units), compared with those of the masing H_2O $5_{1,5}$–$4_{2,2}$ line, and of the narrow (Hot Core) CH_3OH line at 325 GHz presented in Cer99. All the maps were obtained with the 10.4 meter telescope of the Caltech Submillimeter Observatory.

maps: they identify the emission as mainly coming from the Hot Core rather than the Plateau, as we conclude from our lines based on line shape and line width considerations. This discrepancy calls for an explanation that we will provide in the following section.

3. MODEL RESULTS AND DISCUSSION

According to the aperture synthesis maps of the 80.6 GHz HDO emission in Orion-KL performed by Plambeck & Wright (1987) using a synthesized beam of 3″.4, the Plateau emission is marginally detected and the bulk of the emission near IRc2 originates from the Hot Core clump. Since we do not see a clear Hot Core component in our submillimeter HDO lines (see their quite triangular shape in Fig. 1) we have to assume that the line opacity is too high in the Plateau. This is also what happens with HCN 9–8 and 10–9 (see below). On the other hand, the physical conditions should be such that the opacities of the $1_{1,0} \rightarrow 1_{1,1}$ (80.6 GHz) and $2_{1,1} \rightarrow 2_{1,2}$ (241.6 GHz) HDO lines are sufficiently low to reveal the (observed) Hot Core component.

In order to predict brightness temperatures and opacities for the Plateau component of the emission, derive deuterated water abundances and compare them with the values obtained from the 183 and 325 GHz H_2O lines, we have used an LVG model consisting of a molecular shell, 10^{17} centimeters in diameter, expanding at a constant velocity of 25 km s^{-1}, as in Cer99. Collisional rates for HDO-H_2 were estimated from those of HDO-He as calculated by Green (1989). We have computed the brightness main-beam temperature of the $2_{1,2}$–$1_{1,2}$ and $1_{1,1}$–$0_{0,0}$ HDO transitions and the $3_{1,3}$–$2_{2,0}$ and $5_{1,5}$–$4_{2,2}$ para-H_2O transitions versus the column densities of the two molecular species for different volume densities, $n(H_2)$, and kinetic temperatures, T_K (Fig. 3).

The fact that the two newly observed HDO lines have almost identical intensity (a T_{MB} of about 20 K after correcting for the telescope efficiency in the 800–900 GHz range) puts strong constraints on the physical conditions of the emitting region. Adding to this information the intensity ratio $R \sim 10$–50, between the 183 and 325 GHz para-H_2O lines that we presented in Cer99 (note that the 325 GHz emission is spatially restricted to the Plateau) provides a quite precise picture of the water and monodeuterated water abundance in the Plateau environment around Orion IRc2.

For the model to simultaneously fit the above HDO and $H_2^{16}O$ data, volume densities, $n(H_2)$, below 10^6 cm^{-3} and T_K below 150 K can be ruled out (see Fig. 3). We have indicated on Figure 3 the column density ranges compatible with our observations from which we derive the HDO/H_2O ratio in the environment of Orion IRc2. Assuming $T_K = 200$ K and $n(H_2) = 3 \times 10^6$ cm^{-3} we find for an HDO column density of 5×10^{16} cm^{-2}, main beam brightness temperatures of 19.8 K and 16.4 K for the $2_{1,2}$–$1_{1,1}$ and $1_{1,1}$–$0_{0,0}$ lines, respectively. These values are in very good agreement with our observations if we allow for a 25% beam efficiency. The respective opacities would be 3.7 and 6.7, confirming that

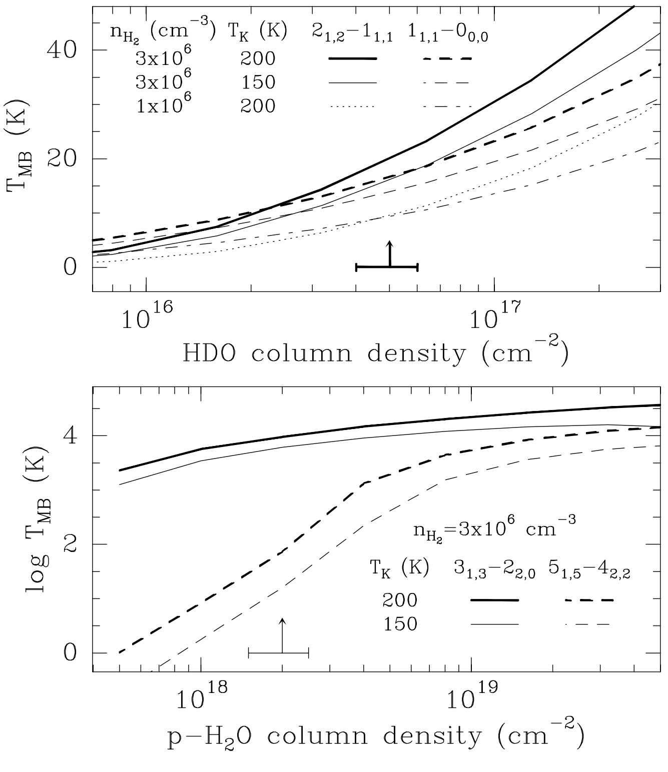

FIG. 3.—Brightness main-beam temperature of the $2_{1,2}$–$1_{1,2}$ and $1_{1,1}$–$0_{0,0}$ HDO transitions and the $3_{1,3}$–$2_{2,0}$ and $5_{1,5}$–$4_{2,2}$ para-H_2O transitions vs. the column densities of the two molecular species, for different values of $n(H_2)$ and T_K. The column density ranges compatible with our observations (Cer99 and this work) are indicated and discussed in the text.

the (foreground) Plateau would hide the Hot Core. In addition, in this case the upper limit for the peak opacity of the millimeter $1_{1,0}$–$1_{1,1}$ and $2_{1,1}$–$2_{1,2}$ HDO transitions would be 1.3 and 0.5, respectively, thus allowing to see the Hot Core (Jacq et al. 1990, using the latter [241.6 GHz] line) or to see evidence of both the Plateau and the Hot Core (Plambeck & Wright 1987 using the former [80.6 GHz] line). The derived HDO column density in the Plateau would be in a rather narrow range of 4–6 × 10^{16} cm^{-2}. In addition, Jacq et al. (1990) saw no Plateau evidence but an important Hot Core signal in the $3_{1,2}$–$2_{2,1}$ line at 225.9 GHz (∼18 K) that is also consistent with the above model: $T_B \leq 0.4$ K for the assumed Plateau conditions, but rapidly increasing to several K as the expansion velocity decreases and the HDO column density and kinetic temperature increase (Hot Core). In addition, the same authors point out that the HDO excitation is strongly controlled by the infrared radiation field. We have incorporated IR dust radiation to our model and have found that this statement is true for many lines observed in Jacq et al. (1990) under the considered conditions, but the effect is less important for our two HDO lines chiefly because both are backbone transitions and their excitation is almost completely dominated by collisions.

Running the same model to fit the observed $J = 9$–8 and $J = 10$–9 HCN lines originating in the Plateau (with a peak in T_{MB} of about 60 K) we find HCN column densities of the order of 2 × 10^{16} cm^{-2}, in very good agreement with the results of Blake et al. (1987): 1.5 × 10^{16} cm^{-2} in the Plateau (and 2.5 × 10^{16} cm^{-2} in the Hot Core). We found that the two HCN lines would under those conditions have peak opacities between 10 and 15, and thus the Hot Core emission, if originating behind, would not be seen as well, as the line profiles suggest. The $J = 8$–7 line of this same molecule at 708.8769 GHz is predicted to be in the same case, and it is confirmed by the results of Schilke et al. (2001). Only the $J = 1$–0 HCN line would be partially transparent to the Hot Core emission (confirmed by the results of Vogel et al. 1985). These results support the idea that the lines of many molecules present in the Plateau become optically thick and then hide the Hot Core emission. Rare isotopes such as $HC^{15}N$ could, however, show a Hot Core feature (see the results of Schilke et al. 2001).

The values of $n(H_2)$ and T_K necessary to explain the spatial peaks of the measured HDO emission leave a very narrow margin of para-H_2O column density compatible with the observed para-H_2O emission at 183 and 325 GHz presented in Cer99. That column density should be in the range 1.5–2.5 × 10^{18} cm^{-2}. As pointed out in Cer99, the widespread emission from the Plateau observed at 183 and 325 GHz is only compatible with more moderate values of $n(H_2)$ and T_K, but since HDO is considerably less extended we are possibly comparing here regions of higher densities and temperatures and thus the values given above would make sense. We would then have a ratio $[HDO]/[H_2O]$ in the range 0.004–0.01 in the Plateau. It can be argued that the $H_2^{18}O$ lines are a better tool than the two para-H_2O transitions used in Cer99 to derive H_2O column densities for comparisons with our HDO data. Jacq et al. (1988) used 203 GHz observations of $H_2^{18}O$ to derive H_2O column densities that suffer from an important blend with SO_2 signal, and this is an even greater drawback than the masing nature of the 183 and 325 GHz H_2O transitions. In addition, although weak, the 203 GHz $H_2^{18}O$ transition could also be maser in nature in some cases (note that this transition is the equivalent of the 183 GHz line of $H_2^{16}O$). But the most important point we want to make here is that the considered para-H_2O transitions allow an estimate of H_2O column densities in the Plateau (Cer99) provided that an appropriate model is used (Cer99), whereas the 203 GHz $H_2^{18}O$ transition in Jacq et al. (1988) only traces the Hot Core (after a careful removal of the SO_2 signal they determine $n(H_2O) < 6.7 \times 10^{18}$ cm^{-2} and a lower limit for $[HDO]/[H_2O]$ of 10^{-3}).

The deuterium enrichment in water thus remains about 1 order of magnitude lower than the one found for methanol. Mauersberger et al. (1998) found CH_3OD/CH_3OH in the range 0.01 to 0.06, Jacq et al. (1993) found CH_2DOH/CH_3OH to be 0.04.

Models using gas-phase molecular chemistry (Millar, Bennett, & Herbst 1989) show that relatively important (even a factor of ∼100) deuterium enhancements can be expected in the molecular content of low-temperature interstellar clouds (below ∼70 K). The most prevalent reaction responsible for deuterium fractionation at low temperatures is the following:

$$H_3^+ + HD \rightleftharpoons H_2D^+ + H_2 ,$$

since it strongly favors the formation of the ion H_2D^+ that will enter then in other chemical routes that will enrich the gas in deuterated molecules, such as HDO. The reaction rate coefficient for the left to right reaction is 9 orders of magnitude larger than that of the backward reaction at 10 K. Although the reaction barrier becomes easier to penetrate as temperature increases, it is not until it reaches 70 K that the difference becomes smaller than 1 order of magnitude. At the same time, a large fraction of molecules (and their deuterated species) are known to stick to dust grains when colliding with them, thus forming an icy mantle. For example, Moneti, Cernicharo, & Pardo (2001) have determined that H_2O is almost entirely (∼99%) frozen onto dust grains in extremely cold ($T_K \sim 10$ K) molecular clouds that intersect the line of sight toward Sgr A*.

For the physical conditions in Orion IRc2, gas-phase models give D/H molecular ratios totally incompatible with the high HDO/H_2O we see by comparing submillimeter HDO lines with 183 and 325 GHz H_2O line emission toward this source. The most widely accepted explanation for the large molecular D/H fractionation ratios in the Orion IRc2 and other Hot Core environments is that the deuterium rich ice mantles formed, as explained in the previous paragraph, in a much colder and collapsing phase and were evaporated following the switch-on of a massive star. Important support to this scenario has been obtained by Roueff et al. (2000) with the discovery of the first doubly deuterated species (ND_2H) in a cold dense core (L134N). Previously, the grain origin of deuterated species in Hot Cores was strengthened by the detection of doubly deuterated formaldehyde in Orion by Turner (1990) and the young protobinary system IRAS 16293−2422 by Ceccarelli et al. (1998). This evaporation also enriches the gaseous medium in H_2O by a factor of ∼100 leading to the strong water emission, supported by observational evidence toward Orion IRc2 (Cer94; Cer99). Recent studies on Hot Core deuterium chemistry (Rodgers & Millar 1996) conclude that the D/H ratios of molecules injected from the dust mantles to the hot gaseous medium do not suffer significant modifications and would then represent those of the original mantles for molecules that were efficiently deposited during the cold phase (such as water and methanol).

4. SUMMARY

HDO hig-resolution mapping using lines above 800 GHz involving low-lying energy levels is now possible with ground-based telescopes, providing an important tool to study the high HDO/H_2O ratio observed in warm molecular clouds such as the environment of Orion IRc2.

Our observations show that HDO emission in two backbone consecutive HDO transitions above 800 GHz toward Orion IRc2 is quite compact (HPW 15″), and it arises mainly from the 20–25 km s^{-1} Plateau, contrary to several other millimeter lines of the same molecule used in earlier works. The IR radiation field plays an important role in the pumping of H_2O and HDO. However, the lines observed in this work connect the lowest backbone levels which are mainly pumped through collisions under the considered physical conditions. The total column density of HDO has been estimated to be in the range $4–6 \times 10^{16}$ in the Plateau implying a ratio with H_2O of 0.004–0.01, a value that supports the idea that the HDO we see was formed at a much earlier time when the cloud was much colder and it has been released from dust grain mantles after the switch-on of IRc2.

Special care has to be taken in the interpretation of the submillimeter and far infrared spectra of Orion as the emission from the core could be blocked for many molecules in the intermediate-velocity gas. Our HDO lines are a clear example of this situation.

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