

Letter to the Editor

H_2^{18}O in hot dense molecular cloud cores

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SUMMARY. We have used the Kitt Peak 12-m telescope to observe the $3_{13}-2_{20}$ line (203407 MHz) of para- H_2^{18}O towards several hot dense sources of molecular line emission. We detect a feature at the correct frequency towards Orion-KL, G34.3+0.2, Sgr B2(N), and W51 e_1/e_2 . The problem of blending with emission from other molecular line species is discussed and we conclude that at least in the case of G34.3+0.2, the identification with H_2^{18}O is likely to be correct. Our rough estimates suggest that in these "hot core" regions, water has an abundance relative to H_2 of order 10^{-5} and is thus less abundant than CO. In Orion-KL, we estimate the abundance ratio $[\text{HDO}]/[\text{H}_2\text{O}]$ to be greater than 10^{-3} .

Key Words: Water, Molecular lines, Deuterium Enrichment, Hot cores

I. INTRODUCTION

Water is notoriously difficult to observe under normal interstellar medium conditions. The well known water masers are excited in clumps whose density is orders of magnitude larger than that of normal molecular clouds. The water vapour in our atmosphere prevents us from observing the transitions which one can expect to be excited at the typical temperatures and densities of the molecular gas. Apart from KAO observations therefore (see Waters et al. (1980), Phillips et al. (1980)), our only direct knowledge of interstellar water is under the highly untypical conditions which prevail in the maser regions. While important in themselves (see Genzel (1986) for a discussion), their observation yields no information concerning the molecular cloud water abundance.

On the other hand, theoretical models (see e.g. Brown et al. (1988)) predict that water may have an abundance comparable to that of CO. H_2O is likely to be produced in large quantities in shocked gas and in many circumstances (Takahashi et al. (1983, 1985), Neufeld and Melnick (1987)), is an important coolant. However, the chemical models are very uncertain and a direct determination of the water abundance is needed. This is difficult on the basis of observations of the main isotopic species since the lines should be mostly optically thick. This objection is unlikely to apply to the ^{18}O substituted form of water which is expected to be a factor of 500 less abundant. Moreover, some H_2^{18}O lines are sufficiently shifted in frequency from their H_2O counterparts that they may be observed from earth-bound telescopes. One case in point is the $3_{13}-2_{20}$ line of H_2^{18}O at 203407 MHz which Phillips et al. (1978) claim to have observed towards Orion-KL and DR21(OH) using the 11-m Kitt Peak telescope. The results are somewhat doubtful because of the possibility of interfering lines of other species (like the

$12_{0,12} \rightarrow 11_{1,11}$ transition of SO_2). We decided therefore that it was worthwhile repeating the Phillips et al. observation with a filterbank spectrometer and improved sensitivity.

We were also motivated by recent HDO observations which we have carried out with the IRAM 30-m telescope. These showed rather surprisingly that HDO can be observed towards several of the hot dense molecular cores which one typically finds in high mass star forming regions. This is important because the 2_{20} level of H_2^{18}O is 135 cm^{-1} (195 K) above the ground and has a radiative lifetime of only four seconds. It therefore requires high temperature and high density conditions in order to be excited (see Phillips et al. (1978)). It therefore seemed likely that sources detected in HDO would be good candidates for emission in the H_2^{18}O line. There is considerable evidence for a high HDO/ H_2O ratio towards Orion-KL (see Henkel et al. (1987), Walmsley et al. (1987), Plambeck and Wright (1987), Mauersberger et al. (1988)) and a direct comparison of the HDO and H_2^{18}O column densities is obviously desirable. In the present article, we discuss H_2^{18}O observations which we have carried out with the NRAO 12-m telescope and in a forthcoming publication, we will present our results for HDO.

II. OBSERVATIONS

H_2^{18}O measurements at 203 GHz were obtained in December 1987 using the NRAO 12-m telescope in Kitt Peak, Arizona¹. The HPBW was 30 arc sec. and the beam efficiency 0.5. We used two receivers equipped with Schottky mixers (effective system temperature 2000–3000 K) operated in double sideband mode and accepting opposite senses of linear polarisation. The observing time per source was divided into two halves with different central velocities in order to allow an assessment of the importance of interfering lines from the image sideband (the image band was centered at 200.383 GHz). The observations were carried out in the position switching mode with a reference position typically offset 1 degree from the source. Pointing checks were carried out on Jupiter and Saturn and we estimate the error to be at most 5 arc sec (10 for G34.3+0.2). We calibrated our data using a chopper vane at ambient temperature and should have errors of less than thirty percent. The spectrometer consisted of two filter banks of $256 \times 1 \text{ MHz}$ and $256 \times 500 \text{ kHz}$ (or occasionally $256 \times 250 \text{ kHz}$) channels which were operated simultaneously. Each bank was split into two sub-blocks of 128 channels set at the same central frequency but

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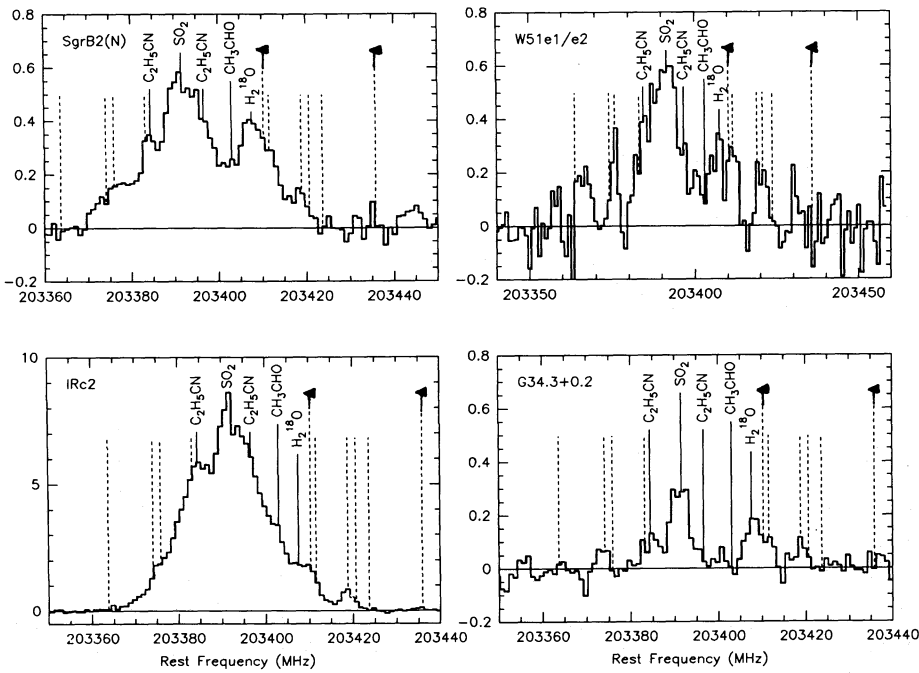


Figure 1: 1 MHz resolution spectra of the H_2^{18}O $3_{13}\rightarrow 2_{20}$ line towards Sgr B2(N), W51(e1/e2), Ori IRc2, and G34.3+0.2. The rest frequencies of various lines discussed in the text are marked by vertical lines. The dashed vertical lines are for dimethyl-ether $(\text{CH}_3)_2\text{O}$ or, when marked by a filled triangle, for methyl formate HCOOCH_3 .

accepting data from the two receivers. Our velocity resolution varied between 0.4 km s^{-1} (250 kHz) and 1.5 km s^{-1} (1 MHz) and our velocity coverage (with the 1 MHz filters) was $\pm 94 \text{ km s}^{-1}$.

III. RESULTS

In Table 1, we summarize the observed positions and the R.M.S. noise levels which we achieved. In Figure 1, we show those spectra for which line emission was observed at the H_2^{18}O line frequency (203407.52 MHz; De Lucia et al. (1972)). It is clear from Figure 1 that there is a considerable likelihood of misidentification of features observed in this frequency range. Tests with shifted local oscillator frequency suggest that essentially all of the emission visible on Figure 1 comes from the signal sideband but, unfortunately, we cannot entirely rule out low-level contamination from the image. Concerning the features observed by Phillips et al. (1978), we do not confirm the rather marginal feature which they observed towards DR21(OH). On the other hand, the emission (mainly due to the $12_{0,12}-11_{1,11}$ line of SO_2) which they observed towards Orion-KL ($T_A^* \sim 0.7 \text{ K}$) is surprisingly weak given the strength ($\sim 2 \text{ K}$ in T_R units) of the emission which we observe at the H_2^{18}O line frequency.

Table 1: Source positions and noise levels for the H_2^{18}O 203.4 GHz observations

Source	$\alpha(1950)$	$\delta(1950)$	V_{LSR} (km s^{-1})	σ_{RMS}^a (K)	Detection (Y/N)
W3(OH)	2 ^h 23 ^m 16.4	61 ^o 38'56"	-44	.05	N
ORI-IRc2	5 32 47	-5 24 24	7	.09	Y
M82	9 51 43	69 54 59	200	.03	N
Sgr B2(N)	17 44 10.6	-28 21 19	60	.03	Y
W31C	18 07 30	-19 56 30	-1	.09	N
G34.3+0.2	18 50 46.2	1 11 13	60	.04	Y
W51D	19 21 22	14 25 14	60	.06	N ^{b)}
W51e1/e2	19 21 26.3	14 24 36	60	.09	Y
DR21(OH)	20 37 18.8	42 11 59	-2	.06	N

a) given for a 1 MHz channel

b) a line was observed during a recent run

More important however is that one can conclude from Figure 1 that, towards each of the four sources, there is evidence for a separate feature at a frequency which agrees well with that expected for H_2^{18}O at the source velocity. Since there is only a single line, this is far from being a convincing identification and we consider our results as giving upper limits to the H_2^{18}O line intensity. On the other hand, we have observed HDO from all of these sources and hence it is quite reasonable that the features seen by us may in fact be due to H_2^{18}O . A fraction of the observed intensity in several sources is however due to blending with known lines. We attempt to assess the importance of this in what follows.

Apart from the SO_2 line mentioned earlier, possible blending lines (see Lovas (1984)) are a pair of methyl formate (HCOOCH_3) lines at 203410.246 MHz ($24_{19,5}\rightarrow 25_{18,8}\text{A}$ and $24_{19,6}\rightarrow 25_{18,7}\text{A}$) as well as the dimethyl ether $((\text{CH}_3)_2\text{O})$ $3_{30}\rightarrow 2_{21}\text{AE}$ transition at 203411.52 MHz. All of these molecules are known to be abundant in Orion-KL and hence, a priori, one might expect them to be present in the other sources also. Less important probably is the acetaldehyde CH_3CHO transition at 203402.969 MHz ($10_{2,8}\rightarrow 10_{0,10}$) since CH_3CHO has an abundance below $2 \cdot 10^{-10}$ (relative to H_2) in the Orion ridge (see Irvine et al. (1987)) and since also, we see no convincing evidence for this line.

The importance of the methyl formate blend can roughly be assessed by examining our spectra for the presence of the $19_{8,11}\rightarrow 19_{7,12}$ line at 203435.832 MHz which was also within our passband. This transition has an excitation of 100.8 cm^{-1} and a line strength of 9.5 as compared with an excitation of 282.5 cm^{-1} and line strength of 0.44 for the lines at 203410.246 MHz (Lovas (1984)). We observe no line at the $19_{8,11}\rightarrow 19_{7,12}$ frequency towards the four sources of Figure 1 and conclude that contamination by methyl formate can be neglected (however for Orion-IRc2, this is questionable - see below).

Analysis of dimethyl-ether in our spectra is also aided by the fact that we observe several lines of this species. The $3_{30}\rightarrow 2_{21}\text{AE}$ line, which is blue-shifted 5.9 km s^{-1} relative to H_2^{18}O , is one of a group of four

Table 2: Observed line parameters in the H_2^{18}O $3_{13} \rightarrow 2_{20}$ line.

Source	1 MHz data				500 kHz/250 kHz data ^{a)}			
	$\int T_{\text{R}}^* dv$ (K km/s)	V_{LSR} (km/s)	Δv (km/s)	T_{R}^* (K)	$\int T_{\text{R}}^* dv$ (K km/s)	V_{LSR} (km/s)	Δv (km/s)	T_{R}^* (K)
ORI-IRC2	<11.2	4.2(.1)	6.7(.3)	1.6	3.1(1.6) 7.4(1.7)	8.0(.7) 4.0(.5)	3.1(1) 4.3(.9)	.9 1.6 ^{b)}
Sgr B2(N)	2.7(.2)	64.8(.5)	7.7(.7)	.3	3.8(.9)	63.6(.8)	9.6(2.4)	.4
G34.3+0.2	1.2(.2)	57.3(.5)	6.2(1.2)	.2	1.1(.1)	57.2(.3)	5.2(.6)	.2
W51e1/e2	2.6(.6)	58.5(.8)	8(2.3)	.3	1.0(.1)	57.4(.1)	2.3(.2)	.4

Notes: a) 250 kHz data for ORI-IRC2, 500 kHz for other sources

b) line parameters for the 4 km/s component

$3_{30} \rightarrow 2_{21}$ lines whose relative intensities in the optically thin limit are expected to be 6.0 (203411.52):10.0 (203418.82) : 6.56 (203420.63) : 1.2 (203423.66) where the respective frequencies are given in parentheses. By fitting the three high-frequency lines, we can obtain a good estimate for the 203411.52 MHz line (or an upper limit to its intensity) and subtract its contribution (which is minor) from H_2^{18}O .

Judging from Figure 1, blending with the 203391.488 MHz line of SO_2 is certainly a problem towards Orion-IRC2, perhaps a problem towards Sgr B2(N) and W51, and can be neglected towards G34.3+0.2. We note that in cases where blending with the SO_2 line is a problem, it is broader than the feature which we identify with H_2^{18}O and hence a reasonable guess at its form can be made. We have therefore subtracted the 203391 MHz SO_2 line where possible and have made gaussian fits to our profiles taking account of the di-methyl ether line mentioned above. The line parameters for " H_2^{18}O " derived in this way are given in Table 2. Parameters derived from both the 1 MHz and 250 or 500 kHz banks are compared in order to help judge the reliability of the results. The values given in Table 2 are, in our view, quite reliable for G34.3+0.2 and should be treated with varying degrees of caution for other sources due to the blending problems discussed earlier. The case of Orion-KL is a special one which we will examine in more detail below. But we stress again that the parameters in Table 2 are upper limits in the sense that there is no definitive proof of an identification with H_2^{18}O .

One can pose the question of the probability of chance coincidence with our H_2^{18}O features based upon the statistics of lines observed by us at intensities comparable to our noise levels. In the spectrum of G34.3+0.2, the SO_2 line and the " H_2^{18}O " line are the only two features clearly out of the noise (i.e. intensity greater than $3\sigma=0.12$ K from Table 1). For a typical line width of 5 MHz (7 km s⁻¹), these two lines occupy only 8 percent of the band observed by us. On the other hand, the H_2^{18}O velocity derived (see Table 2) for G34.3+0.2 differs by 1.6 km s⁻¹ (1.1 MHz) from the mean velocity of NH_3 lines observed by Henkel et al. (1987a) towards this source. For the two HDO lines which we have observed at the 30-m ($4_{22} \rightarrow 4_{23}$ at 143.7 GHz and $3_{12} \rightarrow 2_{21}$ at 225.9 GHz), the difference between the " H_2^{18}O " and the HDO velocities are 0.4 and 0.3 km s⁻¹ respectively. This appears to us to be a relatively convincing coincidence but clearly more proof is needed. For other sources, the evidence is less convincing and we only mention further the case of Orion-KL.

In Orion, the main problem is posed by the wing of the broad SO_2 line. In Figure 2, we show our somewhat subjective eye-estimate of the shape of this line superposed on our spectrum with 250 kHz resolution. This shape is the sum of two gaussian profiles centered at 14.1 km/s and 29.8 km/s. We subtracted this from the observed spectrum and obtain the residual shown in the inset to Figure 2. This residual spectrum shows two blended components with velocities (H_2^{18}O scale) of 8

and 4 km s⁻¹. There is also a small contribution to the profile from the $3_{30} \rightarrow 2_{21}$ AE line of $(\text{CH}_3)_2\text{O}$ mentioned earlier which however can be estimated on the basis of the three other $3_{30} \rightarrow 2_{21}$ lines. The parameters from our fit to the residual spectrum are given in Table 2 where we provisionally identify the 8 km s⁻¹ feature with " H_2^{18}O ". The source of the stronger 4 km s⁻¹ feature is a puzzle. For the reasons discussed earlier, we find an identification with methyl formate implausible although the frequency coincidence is excellent. The emission could also be due to "hot core H_2^{18}O ". High excitation ammonia and other hot core lines typically emit at velocities of 5–6 km s⁻¹ (see e.g. Johansson et al. (1984), Hermsen et al. (1988)). We tentatively conclude (see Table 2) that there is evidence for a 3 km s⁻¹ wide H_2^{18}O line towards Orion-IRC2 with a velocity of 8 km s⁻¹. From our 1 MHz data, we find that, after subtracting SO_2 , a conservative upper limit to the integrated intensity in the H_2^{18}O line is 11 K km s⁻¹.

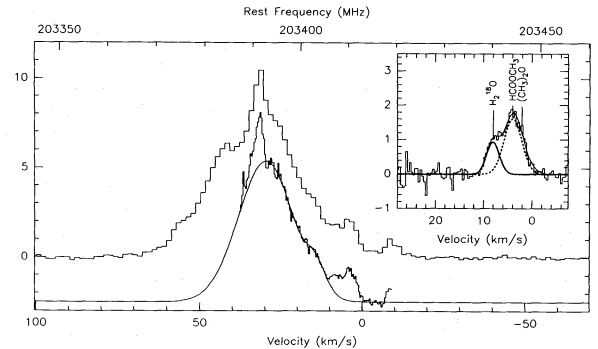


Figure 2. 1 MHz and 250 kHz resolution spectra of the SO_2 - H_2^{18}O blend towards Orion-IRC2 showing (on the 250 kHz spectrum) our suggested fit to the $12_{0,12} \rightarrow 11_{1,11}$ SO_2 line. The 3 component fit made to the residual spectrum after the subtraction of SO_2 is shown on the inset to the figure.

IV. DISCUSSION

For an L.T.E. distribution of level populations, the fraction of H_2^{18}O molecules in the 2_{20} state is given by: $f(2_{20}) = 148 \exp(-194/T_{\text{R}})/T_{\text{R}}^{1.5}$. Here, we have assumed that only a quarter of the H_2^{18}O molecules are of the para variety and have applied the classical partition function. T_{R} is the rotation temperature describing the level populations. One sees that for T_{R} between 50 and 500 K, $f(2_{20})$ only varies between 0.008 and 0.022. Since the rotation temperatures derived from our HDO measurements for the sources observed by us in H_2^{18}O are of order 100 K, it is reasonable to assume $T_{\text{R}}(\text{H}_2^{18}\text{O})$ to have this value and hence $f(2_{20}) \approx 0.02$.

On the other hand, assuming optically thin conditions and a line excitation temperature much larger than 3 K, we have for the beam averaged column density in the 2_{20} level in cm^{-2}

$$N(2_{20}) = 1.2 \cdot 10^{13} \int T_R^* dv / f_B$$

Here, $\int T_R^* dv$ is the integrated line intensity in K km s^{-1} and f_B is the conversion factor to main beam brightness temperature. Taking $f_B=0.5$ (correct for a point source) and a ratio of 500 for $\text{H}_2^{16}\text{O}/\text{H}_2^{18}\text{O}$, we derive the column densities given in Table 3. For the reasons discussed earlier, these should be treated as upper limits.

Table 3: Estimated water and molecular hydrogen beam averaged column densities.

Source	$N(2_{20})$ cm^{-2}	$N(\text{H}_2\text{O})^*$ cm^{-2}	$N(\text{H}_2)$ cm^{-2}	Ref. for $N(\text{H}_2)$
ORI-IRC2	$<2.7 \cdot 10^{14}$	$<6.7 \cdot 10^{18}$	$3.0 \cdot 10^{23}$	1
Sgr B2N	$6.5 \cdot 10^{13}$	$1.6 \cdot 10^{18}$	$2 \cdot 10^{23}$	2,3
G34.3+0.2	$2.9 \cdot 10^{13}$	$7.2 \cdot 10^{17}$	10^{23}	4,5
W51e1/e2	$6.2 \cdot 10^{13}$	$1.6 \cdot 10^{18}$	$<10^{24}$	6,7

References for H_2 column densities:

1. Keene et al. (1982)
2. Irvine et al. (1987)
3. Goldsmith et al. (1987)
4. Heaton et al. (1985)
5. Henkel et al. (1987a)
6. Jaffe et al. (1984)
7. Cunningham et al. (1984)
- * Assuming $\text{H}_2\text{O}/\text{H}_2^{18}\text{O}=500$

In Table 3, we also give hydrogen column densities averaged over a $30''$ beam for the sources of interest. Here, it is important to realise that only the relatively hot (>50 K) dense gas contributes to the observed H_2O emission and hence, one must compare our observed water column densities with the hot hydrogen column density along the line of sight. Column densities derived from CO or 1-mm dust emission are liable to be irrelevant except perhaps for Ori-IRC2. Moreover, interferometer observations have made it clear that all of our sources contain considerable structure on size-scales much smaller than our angular resolution. We have made educated guesses based upon the literature references cited in Table 3 in order to derive hydrogen column densities. We conclude tentatively that the water abundance in the hot regions studied by us is probably of order 10^{-5} and almost certainly not greater than the Ori-IRC2 upper limit of $2 \cdot 10^{-5}$. Thus in these sources at least, water appears to be less abundant than CO which has typically an abundance of order 10^{-4} . However one should note that the estimates in Table 3 represent averages over our beam and we certainly cannot exclude the possibility of clumps within the beam having different abundances.

Our results also confirm the conclusion (Plambeck and Wright (1987), Henkel et al. (1987b)) that the $\text{HDO}/\text{H}_2\text{O}$ abundance ratio in the Orion hot core is much greater than the interstellar D/H ratio of $\sim 10^{-5}$. Combining our limit for H_2O in Orion-KL with the HDO column density from Henkel et al. (1987b) (corrected to a beam of $30''$), we derive a lower limit to $[\text{HDO}]/[\text{H}_2\text{O}]$ of 10^{-3} . Thus water in Orion-KL is enriched in deuterium by at least a factor of 100. Since shocks are not expected to cause HDO enhancement (see Moore et al., 1986), one concludes that much of the observed H_2O emission towards Orion-KL is not due to shock processing. However, our observations are not very sensitive to weak broad plateau-like lines and that we could not detect in Orion, for example, a 50 km s^{-1} wide line of strength 0.2 K. This gives roughly the same column density limit as in Table 3.

It is worth noting that the sources in which we have tentatively detected H_2^{18}O are the same sources

in which HDO has been found. Conversely, our negative results are in sources where HDO has not yet been detected. It is attractive to interpret this in terms of evaporation from grain mantles as has been done for Orion (see Plambeck and Wright (1987), Henkel et al. (1987b)). Brown et al. (1988) have modelled a situation in which previously accreted ice mantles are evaporated due to the switch-on of a young massive star as in the Orion hot core. They predict an abundance of $4.7 \cdot 10^{-4}$ for $\text{H}_2\text{O}/\text{H}_2$ which is in fact much more than what we calculated above. This suggests that oxygen in grain mantles may be in other forms than water ice. In fact, Tielens and Allamandola (1987) suggest on the basis of infrared measurements that solid CH_3OH may be as abundant as solid H_2O . Hence, the problem with the models may be lack of understanding of dust mantle chemistry.

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