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Water abundance in molecular cloud cores

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WATER ABUNDANCE IN MOLECULAR CLOUD CORES


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ABSTRACT

We present Submillimeter Wave Astronomy Satellite (SWAS) observations of the $1_{0} \rightarrow 1_{01}$ transition of ortho-$\text{H}_2^{16}$O at 557 GHz toward 12 molecular cloud cores. The water emission was detected in NGC 7538, $\rho$ Oph A, NGC 2024, CRL 2591, W3, W3(OH), Mon R2, and W33, and was not detected in TMC-1, L134N, and B335. We also present a small map of the $\text{H}_2^{18}$O emission in S140. Observations of the $\text{H}_2^{18}$O line were obtained toward S140 and NGC 7538, but no emission was detected. The abundance of ortho-$\text{H}_2^{16}$O relative to $\text{H}_2$ in the giant molecular cloud cores was found to vary between $6 \times 10^{-10}$ and $1 \times 10^{-8}$. Five of the cloud cores in our sample have previous $\text{H}_2^{18}$O detections; however, in all cases the emission is thought to arise from hot cores with small angular extents. The $\text{H}_2^{18}$O abundance estimated for the hot core gas is at least 100 times larger than in the gas probed by SWAS. The most stringent upper limit on the ortho-$\text{H}_2^{16}$O abundance in dark clouds is provided in TMC-1, where the 3$\sigma$ upper limit on the ortho-$\text{H}_2^{16}$O fractional abundance is $7 \times 10^{-8}$.

Subject headings: ISM: abundances — ISM: clouds — ISM: molecules — radio lines: ISM

1. INTRODUCTION

The Submillimeter Wave Astronomy Satellite (SWAS) has detected spatially extended $\text{H}_2^{16}$O emission associated with the quiescent dense molecular gas in Orion and M17 (Snell et al. 2000a,b). Based on these observations the relative abundance of ortho-$\text{H}_2$ was found to be surprisingly small, ranging from only $1 \times 10^{-9}$ to $8 \times 10^{-8}$. We present here SWAS observations of the ortho-$\text{H}_2^{16}$O transition at 557 GHz in the three dark cloud cores TMC-1, L134N and B335 and in the nine giant molecular cloud cores W3, W3(OH), Mon R2, $\rho$ Oph A, W33, CRL 2591, S140, and NGC 7538.

Five of the cloud cores in our survey have had previously reported water detections. NGC 7538, S140, W3, and CRL 2591 were detected by the Infrared Space Observatory in the rovibrational lines of $\text{H}_2^{16}$O from the $12\nu$ bending mode at 6 $\mu$m in absorption against the dust continuum (van Dishoeck & Helmeich 1996; Helmich et al. 1996; van Dishoeck 1998). Water emission has also been detected in NGC 7538, W3, and W3(OH) from the $31_3 \rightarrow 2_20$ transition of $\text{H}_2^{16}$O at 183 GHz (Cernicharo et al. 1990) and the $31_3 \rightarrow 2_20$ transition of $\text{H}_2^{18}$O at 203 GHz (Gensheimer, Mauersberger, & Wilson 1996). The 183 GHz and 203 GHz lines arise from transitions with relatively high energies ($E_u/k \gg 200$ K) and thus are likely produced in relatively warm gas. The 6 $\mu$m absorption features can arise from a range of gas temperatures, however the absorption seen in these sources is thought to be dominated by relatively warm gas. The relative abundance of $\text{H}_2^{16}$O in the warm gas has been estimated to be $1 \times 10^{-8}$ to $1 \times 10^{-4}$. SWAS on the other hand, can observe the lowest energy rotational transition of ortho-$\text{H}_2^{16}$O permitting detection of $\text{H}_2^{16}$O emission from the more extended, cold core gas. We estimate the abundance of ortho-water in the relatively cold ($T < 50$ K) core gas and compare the abundance results with those for the warm gas and those for Orion and M17.

2. OBSERVATIONS AND RESULTS

The observations of $\text{H}_2^{16}$O and $\text{H}_2^{18}$O reported here were obtained by SWAS during the period 1998 December to 2000 January. The data were acquired by nodding the satellite alternatively between the cloud core and a reference position free of molecular emission. Details concerning data acquisition, calibration, and reduction with SWAS are presented in Melnick et al. (2000). Observations of the $1_{0} \rightarrow 1_{01}$ transition of $\text{H}_2^{16}$O at a frequency of 556.936 GHz were obtained toward the positions given in Table 1. Total integration times for these observations range from 17 hr for W3(OH) to 127 hr for L134N.

In addition, we obtained a small 10-point map of the S140 cloud core with integration times per position of between 18 and 36 hr. The center positions of S140 and NGC 7538 were also observed in $\text{H}_2^{18}$O at a frequency of 547.676 GHz for 189 and 36 hr respectively. The SWAS beam is elliptical, and at the frequency of the water transitions has angular dimensions of 3.3 $\times$ 4.5'. The data shown in this paper are in antenna temperature units and are not corrected for the measured SWAS main beam efficiency of 0.90. We also used the Five College Radio Astronomy Observatory (FCRAO) 14 m telescope to map the $J=1 \rightarrow 0$ transition of $\text{C}^{18}$O in an approximately 6' $\times$ 6' region in each core to provide an estimate of the gas column density.
for use in our analysis of the H$_2$O data.

H$_2$O emission was detected in all nine giant molecular cloud cores. However despite deep integrations, we were unable to detect H$_2$O emission in any of the three dark cloud cores. The H$_2$O spectra obtained for six of the cloud cores are shown in Figure 1. Spectra for five of the remaining six cores are shown in Ashby et al. (2000a). The spectrum of B335, where no H$_2$O emission was detected, is not shown. The H$_2$O line profiles for the giant molecular cloud cores show a wide variety of shapes, ranging from relatively narrow single-peaked lines to broad, strongly self-absorbed lines. We have marked in Figure 1 the line center velocity of the $^{13}$CO $J = 5 \rightarrow 4$ emission (J. Howe et al. 2000, in preparation) observed simultaneously with SWAS. In W3, Mon R2, and W33 it is obvious that the H$_2$O line is self-absorbed, since the peak of the $^{13}$CO emission corresponds to a minimum in the H$_2$O emission. CRL 2591 is probably also self-absorbed, although in this case the situation is somewhat more ambiguous. More discussion about the H$_2$O line profiles can be found in Ashby et al. (2000a). The spectra for $\rho$ Oph A and NGC 7538 presented in Ashby et al. (2000a) show obvious broad wings, suggesting that some of the H$_2$O emission probably arises in associated molecular outflows.

A small map of the H$_2$O emission in S140 is shown in Figure 2. The emission toward the center of the core reveals a relatively narrow ($\Delta V_{FWHM} = 5.7$ km s$^{-1}$), single-peaked line. H$_2$O emission was also detected at positions 3/2 to the north and south of center, however no emission was found east or west of center. The off-center spectra in general have rms noise of 0.02 K, about 2 times larger than the center position. During these observations the long axis of the SWAS beam was oriented approximately north-south, thus explaining the stronger emission detected in these directions.

We failed to detect H$_{18}$O emission in either S140 or NGC 7538. The rms noise achieved in the NGC 7538 observations of 0.03 K was not adequate to place a very useful limit on the H$_2$O/H$_{18}$O ratio. In S140, however, the H$_{18}$O spectrum had an rms noise of only 0.01 K. In S140 we used the line width and line center velocity derived from a Gaussian fit to the H$_2$O line (see Figure 2) to constrain a Gaussian fit to the H$_{18}$O spectra. From this constrained fit we derived a 1σ upper limit to the integrated intensity of 0.022 K km s$^{-1}$ leading to a 1σ lower limit on the intensity ratio of H$_2$O/H$_{18}$O of 70.

### Table 1

<table>
<thead>
<tr>
<th>Source</th>
<th>R.A. (J2000)</th>
<th>Decl. (J2000)</th>
<th>$\int T_a^d dv$</th>
<th>$\sigma$ ($T_a^d$)</th>
<th>Temperature</th>
<th>log $\epsilon$</th>
<th>$x$(H$_2$O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>W3</td>
<td>02 23 29.9</td>
<td>+62 05 54</td>
<td>2.93</td>
<td>0.13</td>
<td>45</td>
<td>6.0</td>
<td>2x10$^{-8}$</td>
</tr>
<tr>
<td>W3(OH)</td>
<td>02 27 02.8</td>
<td>+61 52 21</td>
<td>2.93</td>
<td>0.13</td>
<td>30</td>
<td>6.3</td>
<td>2x10$^{-8}$</td>
</tr>
<tr>
<td>TMC-1</td>
<td>04 41 20.4</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>NGC 2024</td>
<td>05 41 44.5</td>
<td>-01 55 35</td>
<td>0.83</td>
<td>0.06</td>
<td>35</td>
<td>6.0</td>
<td>$&lt;7x10^{-4}$</td>
</tr>
<tr>
<td>Mon R2</td>
<td>06 07 40.2</td>
<td>-06 23 28</td>
<td>0.90</td>
<td>0.07</td>
<td>40</td>
<td>5.6</td>
<td>$&lt;3x10^{-4}$</td>
</tr>
<tr>
<td>L134N</td>
<td>15 54 06.5</td>
<td>-02 52 19</td>
<td>0.81</td>
<td>0.02</td>
<td>10</td>
<td>4.3</td>
<td>$&lt;1x10^{-6}$</td>
</tr>
<tr>
<td>$\rho$ Oph</td>
<td>16 26 19.3</td>
<td>-24 24 02</td>
<td>0.81</td>
<td>0.02</td>
<td>30</td>
<td>5.5</td>
<td>$&lt;3x10^{-4}$</td>
</tr>
<tr>
<td>W33</td>
<td>18 14 15.1</td>
<td>-17 55 25</td>
<td>0.46</td>
<td>0.08</td>
<td>23</td>
<td>5.7</td>
<td>$1x10^{-4}$</td>
</tr>
<tr>
<td>B335</td>
<td>19 36 58.7</td>
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<td>10</td>
<td>4.3</td>
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<tr>
<td>CRL 2591</td>
<td>20 29 25.9</td>
<td>+40 11 19</td>
<td>0.34</td>
<td>0.04</td>
<td>38</td>
<td>5.1</td>
<td>$6x10^{-8}$</td>
</tr>
<tr>
<td>S140</td>
<td>22 19 17.1</td>
<td>+62 18 46</td>
<td>1.71</td>
<td>0.08</td>
<td>30</td>
<td>5.8</td>
<td>$8x10^{-4}$</td>
</tr>
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<td>NGC 7538</td>
<td>23 13 47.6</td>
<td>+61 26 54</td>
<td>3.09</td>
<td>0.10</td>
<td>25</td>
<td>6.0</td>
<td>$1x10^{-4}$</td>
</tr>
</tbody>
</table>

Note. — Units of right ascension are hours, minutes, and seconds, and units of declination are degrees, arcminutes, and arcseconds.

3. DETERMINATION OF THE WATER ABUNDANCE

We have analyzed the H$_2$O observations of the twelve cores.
in the same manner as reported for Orion and M17 (Snell et al. 2000a, 2000b). Before reviewing this procedure, it is worth noting that the critical density for the 557 GHz transition of H$_2$O observed by SWAS is of order 10$^8$ cm$^{-3}$, much higher than the average density of gas in these cores. Therefore the probability of collisional deexcitation of this transition is very small, and photons produced by collisional excitations will all escape the cloud core, although they may be repeatedly absorbed and reemitted. A linear relation thus exists between the observed line integrated intensity and the product of the density and the ortho-H$_2$O column density, independent of the optical depth of this transition (Linke et al. 1977; Snell et al. 2000a). The emission in this case is effectively optically thin. Although we did not use this analytical expression to derive abundances, it provides insight into the dependence of the water abundance on the physical properties of the cloud.

We estimate the relative ortho-H$_2$O abundance using a simple model of the temperature, density, column density, and velocity dispersion for the gas in each core. The gas column density distribution was determined from the C$^{18}$O maps, sampled at 44$''$ intervals, assuming LTE and a C$^{18}$O/H$_2$ abundance ratio of 1.7 $\times$ 10$^{-7}$. The SWAS beam filling factor is effectively the convolution of the column density distribution with the SWAS beam pattern. The velocity dispersion of the gas along each line of sight was determined from the C$^{18}$O line width. Another important parameter in our modeling is the gas density. For five sources (W3, W3(OH), $\rho$ Oph, W33, and Mon R2) we have strip maps of the CS on $J = 2 \rightarrow 1$ emission obtained at FCRAO and the $J = 5 \rightarrow 4$ and $J = 7 \rightarrow 6$ transitions obtained at KOSMA. Most of this data is unpublished, although the results for the core centers can be found in Trojan (2000). The CS emission was found to be centrally peaked in these cores with detectable emission extending at least several arcminutes from the center. Modeling of these data suggests that even though the column density decreases rapidly away from the core center, the density remains relatively constant. We used the published density results for L134N (Dickens et al. 2000), TMC-1 (Pratap et al. 1997), S140 (Snell et al. 1984; Zhou et al. 1994), NGC 2024 (Snell et al. 1984; Schulz et al. 1991), B335 (Zhou et al. 1993), NGC 7538 (Plume et al. 1997) and CRL 2591 (Carr et al. 1995; van Dishoeck et al. 1999) in our modeling. For L134N, TMC-1, S140, and NGC 2024 these authors have found that the density is relatively constant across the core. Thus for many of the cores the high column density gas, which dominates the SWAS emission, can be roughly characterized by a single density. We therefore assumed a constant density and temperature for the cores, and the values used are summarized in Table 1. Although a single density cannot apply to all of the gas within the SWAS beam, we believe that the use of this approximation should not lead to serious errors in our abundance determinations.

The collisional excitation of H$_2$O was computed using both the para- and ortho-H$_2$ collision rates with ortho-H$_2$O (Phillips, Maluendes, & Green 1996), and assuming a ratio of ortho- to para-H$_2$ given by LTE at the temperatures given in Table 1. We did not include dust in our model, however the calculations of Ashby et al. (2000b) for S140 and $\rho$ Oph A indicate that the exclusion of the dust continuum emission will have only a minor impact on the determination of the water abundance. We do note that in W33, the line is clearly absorbing the dust continuum, and therefore some of the dust continuum photons are converted into line photons. For our analysis we have used the total integrated intensity including the negative contribution in the absorption feature, and thus, the integrated line intensity should be representative of the total number of line photons.

We proceed in our analysis by guessing a relative ortho-H$_2$O abundance for the core, then computing the emission distribution, and finally convolving that distribution with the SWAS beam. The abundance of H$_2$O is varied until the modeled integrated intensity agrees with observations. We assume a constant H$_2$O abundance across each source. For positions with no detections, we used the 3$\sigma$ upper limit on the integrated intensity to establish a 3$\sigma$ upper limit on the H$_2$O abundance. The abundances and/or limits found for each core are given in Table 1. For S140 and $\rho$ Oph A our results agree well with the abundances derived by Ashby et al. (2000b) using a more detailed 3-dimensional model of the density and temperature profile within these sources. The uncertainty in our derived abundances is dominated by the uncertainties in the physical conditions, chiefly density. The accuracy of density determinations is of order a factor of three, thus leading to abundance uncertainties of the same magnitude. However, due to our use of a single density to characterize these cores, the gas density at the periphery of the cloud cores may be overestimated. This does not have a big impact on the abundance determination because the column density is low in these regions and does not contribute substantially to the H$_2$O emission detected by SWAS. Nevertheless, the use of a single density slightly biases our abundance determinations toward lower values.

In the giant molecular cloud cores the abundance of ortho-H$_2$O relative to H$_2$ varies from 6 $\times$ 10$^{-10}$ to 1 $\times$ 10$^{-8}$. The highest H$_2$O abundances are derived for NGC 7538 and S140. The high H$_2$O abundance found for NGC 7538 is in part a consequence of including emission arising from the molecular outflows, thus resulting in an overestimate of the core abundance. However, in S140, the line profile is relatively narrow and it is unlikely that the core emission is substantially contaminated by outflow emission.

We have also analyzed the mapping data for S140 using the same model as used for the center position. The detected H$_2$O emission at positions 3/2 north and 3/2 south of center is consistent with the predictions based on our cloud model using the abundance of H$_2$O found for the core center. The cloud core is extended to the north-east, and the absence of H$_2$O emission toward the positions east and north-east of the core center requires that either the abundance of ortho-H$_2$O or the gas density be about 2 to 4 times smaller than toward the core center. The absence of extended emission in the higher rotational transitions of CS (Snell et al. 1984), suggests that the lack of H$_2$O emission is most likely explained by a lower density and not a lower abundance. The non-detections of H$_2$O emission in the remaining positions is entirely consistent with our cloud model and the H$_2$O abundance reported in Table 1.

Although we believe that for most of the gas the H$_2$O emission is effectively thin, it is possible that there are very small dense knots of gas that are not. In addition, a relatively thin layer of gas in an extended envelope surrounding the core could have sufficient H$_2$O optical depth to scatter the line photons that arise from the core (Snell et al. 2000a). The H$_2^{18}$O line should be less sensitive to these problems since it is optically thin, and therefore a more reliable estimator of the H$_2$O abundance. We have used the H$_2^{18}$O observations toward the S140 core to establish an upper limit to the fractional abundance of ortho-H$_2$O. Using the same physical model described above, we derive a 3$\sigma$ upper limit to the ortho-H$_2^{18}$O abundance of 3 $\times$ 10$^{-10}$. As-
suming a ratio of H$_2$O/H$_{18}$O of 500, this corresponds to a 3σ upper limit of $1 \times 10^{-7}$ for the abundance of ortho-H$_2$O relative to H$_2$. Comparing this result to our estimate of the H$_2$O abundance obtained from the more common isotopic species, it is not surprising that we were unable to detect H$_{18}$O in this core.

We failed to detect H$_2$O emission from the three dark cloud cores observed by SWAS. Although we achieved similar signal-to-noise ratio in all three cores, the higher density and column density in TMC-1 permit establishing a more stringent limit on the ortho-H$_2$O abundance. In TMC-1, we find a 3σ upper limit on the fractional abundance of ortho-H$_2$O of $7 \times 10^{-8}$. However, even in TMC-1 the water abundance limit is nearly two orders of magnitude larger than the typical giant molecular cloud core. The lower density and temperature in dark cloud cores make detection of H$_2$O very difficult.

4. DISCUSSION AND SUMMARY

SWAS has detected thermal water emission from nine giant molecular cloud cores which permit us to make the first estimate of the water abundance in the cold, dense core gas. The abundance of ortho-H$_2$O relative to H$_2$ in these cloud cores varies from $6 \times 10^{-10}$ to $1 \times 10^{-8}$. The relative ortho-H$_2$O abundance in the majority of these cores is of order $1 \times 10^{-8}$, similar to the abundances found for M17SW (Snell et al. 2000b). In S140 the relative abundance of ortho-H$_2$O is about ten times larger, closer to the average ortho-H$_2$O abundance for Orion (Snell et al. 2000a). In general the relative abundance of ortho-H$_2$O found in these cores is inconsistent with chemical equilibrium models of well-shielded regions of clouds (Bergin, Melnick, & Neufeld 1998), even considering the most extreme uncertainties that might arise in our modeling procedure. Possible explanations for this discrepancy are discussed in Bergin et al. (2000).

Water has been previously detected from the hot gas in W3 IRS 5, W3(OH), CRL 2591, S140, and NGC 7538 IRS 1 via the 183 and 203 GHz emission lines and the ro-vibrational absorption lines at 6 μm (van Dishoeck & Helmi 1996; Helmi et al. 1996; Gensheimer et al. 1996; van Dishoeck 1998). It is worth noting that the SWAS observation of W3 is centered about midway between IRS 4 and IRS 5, less than 1′ from IRS 5; and the SWAS observation of NGC 7538 is centered about 1′ south of IRS 1. In both cases the regions probed via the 6 μm, 183 GHz, and 203 GHz transitions are well within the SWAS beam. The water emission and absorption in these cores is thought to arise from hot cores surrounding young, massive stars with angular extents of only a few arcseconds and gas temperatures $\geq 300$ K (van Dishoeck 1998; van Dishoeck et al. 1999). Abundance estimates for water in the hot cores range from $1 \times 10^{-6}$ to $1 \times 10^{-7}$, several orders of magnitude greater than the abundance of water in the surrounding core gas. Even our limit on the H$_2$O abundance based on H$_{18}$O in S140 rules out the possibility that the large H$_2$O abundance found for the warm gas applies to the general cloud core. At temperatures exceeding 200–400 K, found in shocks and hot cores, a series of neutral-neutral reactions rapidly converts nearly all of the gas phase oxygen into water (Charnley 1997; Bergin et al. 1998). Thus, the substantial difference predicted by the gas-phase chemistry models for the water abundance in warm and cold gas is confirmed by our observations.

SWAS, with a large beam size and the ability to observe a low excitation line of water, is most sensitive to the water emission from the extended, colder dense gas. However, if the water abundance in the cold gas is extremely small, then the hot cores may still contribute to the emission seen by SWAS. If we assume that the brightness temperature of the 557 GHz emission from the hot core gas is 300 K (the same excitation temperature as implied by the absorption lines seen by Infrared Space Observatory) and that the core has an angular size of at most 2′, then the contribution to the observed SWAS H$_2$O emission is negligible in most sources, except CRL 2591. Although van der Tak et al. (1999) suggest that the CRL 2591 hot core has an angular diameter much less than 1′′, the extremely weak emission detected in this source could have a significant hot-core contribution. Further information on the temperature and angular size of the hot core is needed to evaluate this possibility. If a significant fraction of the water emission detected by SWAS in CRL 2591 is attributed to the hot core, then the abundance of H$_2$O in the cold gas is even smaller than that quoted in Table 1.

Only upper limits to the ortho-H$_2$O abundance could be established for the dark cloud cores. If the abundance of water in these cores is as small as that found for the giant molecular cloud cores, it will be difficult to detect water emission in quiescent dark cloud cores. The most stringent limit on the ortho-H$_2$O abundance is set in TMC-1, and in this core the 3σ upper limit on the H$_2$O abundance is just marginally consistent with equilibrium gas-phase chemistry predictions (Bergin et al. 2000). B335 is the site of a well-studied class 0 protostar, while neither L134N nor TMC-1 are actively forming stars. Broad H$_2$O emission has been detected by SWAS toward two other class 0 protostellar cores, L1157 and NGC 1333 IRAS 4 (Neufeld et al. 2000). The H$_2$O emission in these sources clearly arises from the molecular outflows associated with class 0 sources. The relative abundance of ortho-H$_2$O in the outflow gas found by Neufeld et al. (2000) is of order $1 \times 10^{-6}$, considerably larger than the limit set in the two non-star forming cores, L134N and TMC-1. Neufeld et al. (2000) suggests that the enhanced abundance is due to shocks that convert a large fraction of the gas-phase oxygen into water. B335 also has an associated molecular outflow, with a outflow mass between that of L1157 and NGC 1333 IRAS 4 (Moriarty-Schieven & Snell 1989; Neufeld et al. 2000). The absence of H$_2$O emission in B335 is difficult to understand, unless either the density of the outflow gas is much lower than in L1157 or NGC 1333 IRAS 4, or the shock velocities are sufficiently small that H$_2$O formation by neutral-neutral reactions is inhibited.

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