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WATER ABUNDANCE IN MOLECULAR CLOUD CORES

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AND G. J. MELNICK² Received 2000 March 27; accepted 2000 June 21; published 2000 August 16

ABSTRACT

We present Submillimeter Wave Astronomy Satellite (SWAS) observations of the $1_{10} \rightarrow 1_{01}$ transition of ortho-H₂O at 557 GHz toward 12 molecular cloud cores. The water emission was detected in NGC 7538, ρ 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 H_2O emission in S140. Observations of the $H_2^{18}O$ line were obtained toward S140 and NGC 7538, but no emission was detected. The abundance of ortho-H2O relative to H2 in the giant molecular cloud cores was found to vary between 6×10^{-10} and 1×10^{-8} . Five of the cloud cores in our sample have previous H₂O detections; however, in all cases the emission is thought to arise from hot cores with small angular extents. The H_2O 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-H₂O abundance in dark clouds is provided in TMC-1, where the 3σ upper limit on the ortho-H₂O fractional abundance is 7×10^{-8} .

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

1. INTRODUCTION

The Submillimeter Wave Astronomy Satellite (SWAS) has detected spatially extended H₂O 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-H₂O was found to be surprisingly small, ranging from only 1×10^{-9} to 8×10^{-8} . We present here SWAS observations of the ortho-H₂O 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, *ρ* 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 H₂O from the ν_2 bending mode at 6 μ m in absorption against the dust continuum (van Dishoeck & Helmich 1996; Helmich et al. 1996; van Dishoeck 1998). Water emission has also been detected in NGC 7538, W3, and W3(OH) from the $3_{13} \rightarrow 2_{20}$ transition of H₂O at 183 GHz (Cernicharo et al. 1990) and the $3_{13} \rightarrow 2_{20}$ transition of $H_2^{18}O$ at 203 GHz (Gensheimer, Mauersberger, & Wilson 1996). The 183 GHz and 203 GHz lines arise from transitions with relatively high energies ($E_u/k \gtrsim 200$ K) and thus are likely produced in relatively warm gas. The 6 μ 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 H₂O in the warm gas has been estimated to be 1×10^{-6} to 1×10^{-4} . SWAS, on the other hand, can observe the lowest energy rotational transi-

tion of ortho-H₂O permitting detection of H₂O 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 H₂O and H¹⁸₂O 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 $1_{10} \rightarrow 1_{01}$ transition of H₂O 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 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 C¹⁸O in an approximately 6' × 6' region in each core to provide an estimate of the gas column density

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WATER ABUNDANCE IN MOLECULAR CLOUD CORES

TABLE 1							
WATER LINE PARAMETERS AND ABUNDANCE DETERMINATION							

Source	R.A. (J2000)	Decl. (J2000)	$\int T_A^* dv$ (K km s ⁻¹)	$\frac{\sigma(\int T_A^* dv)}{(\mathrm{K \ km \ s}^{-1})}$	Temperature (K)	$\log n \\ (\rm cm^{-3})$	<i>x</i> (o-H ₂ O)
W3	02 25 29.9	+62 05 54	2.93	0.13	45	6.0	2×10^{-9}
W3(OH)	02 27 02.8	+61 52 21	2.93	0.13	30	6.3	2×10^{-9}
TMC-1	04 41 20.4	+25 47 52		0.02	10	4.8	$< 7 \times 10^{-8}$
NGC 2024	05 41 44.5	-01 55 35	0.83	0.06	35	6.0	6×10^{-10}
Mon R2	06 07 40.2	-06 23 28	0.90	0.07	40	5.6	2×10^{-9}
L134N	15 54 06.5	-02 52 19		0.02	10	4.3	$< 3 \times 10^{-7}$
ρ Oph	16 26 19.3	-24 24 02	0.81	0.05	30	5.5	3×10^{-9}
W33	18 14 15.1	-17 55 25	0.46	0.08	23	5.7	1×10^{-9}
B335	19 36 58.7	+07 33 47		0.02	10	4.3	$< 1 \times 10^{-6}$
CRL 2591	20 29 25.9	+40 11 19	0.34	0.04	38	5.1	6×10^{-9}
S140	22 19 17.1	+62 18 46	1.71	0.08	30	5.8	8×10^{-9}
NGC 7538	23 13 47.6	+61 26 54	3.09	0.10	25	6.0	1×10^{-8}

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

for use in our analysis of the H₂O data.

H₂O emission was detected in all nine giant molecular cloud cores. However despite deep integrations, we were unable to detect H₂O emission in any of the three dark cloud cores. The H₂O 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_2O emission was detected, is not shown. The H₂O 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 ¹³CO $J = 5 \rightarrow 4$ emission (J. Howe et al. 2000, in preparation) observed simultaneously with SWAS. In W3, Mon R2, and W33 it is obvious that the H₂O line is selfabsorbed, since the peak of the ¹³CO emission corresponds to a minimum in the H₂O emission. CRL 2591 is probably also self-absorbed, although in this case the situation is somewhat more ambiguous. More discussion about the H₂O line profiles can be found in Ashby et al. (2000a). The spectra for ρ Oph A and NGC 7538 presented in Ashby et al. (2000a) show obvious broad wings, suggesting that some of the H₂O emission probably arises in associated molecular outflows.

A small map of the H_2O emission in S140 is shown in Figure 2. The emission toward the center of the core reveals a rela-



FIG. 1.— Spectra of the $1_{10} \rightarrow 1_{01}$ transition of ortho-H₂O from six cloud cores. The line center velocity of the ¹³CO $J = 5 \rightarrow 4$ transition observed simultaneously with *SWAS* is indicated for W3, Mon R2, CRL 2591, and W33 by a dotted line. The coordinates of each core are given in Table 1.

tively narrow ($\Delta V_{FWHM} = 5.7 \text{ km s}^{-1}$), single-peaked line. H₂O 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 $H_2^{18}O$ emission in either S140 or NGC 7538. The rms noise achieved in the NGC 7538 observation of 0.03 K was not adequate to place a very useful limit on the $H_2O/H_2^{18}O$ ratio. In S140, however, the $H_2^{18}O$ 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_2O line (see Fig. 2) to constrain a Gaussian fit to the $H_2^{18}O$ 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 $H_2O/H_2^{18}O$ of 70.

3. DETERMINATION OF THE WATER ABUNDANCE

We have analyzed the H₂O observations of the twelve cores



FIG. 2.— 10-position map of the $1_{10} \rightarrow 1_{01}$ transition of ortho-H₂O obtained with *SWAS* toward S140. The spectra were obtained on a regular grid spaced by 3'2 and are shown in their correct relative positions on the sky. Offsets in arcminutes relative to the position of S140 given in Table 1 are indicated for each spectrum.

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_2O 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-H₂O 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-H2O 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 C¹⁸O maps, sampled at 44" intervals, assuming LTE and a $C^{18}O/H_2$ abundance ratio of 1.7×10^{-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 C¹⁸O line width. Another important parameter in our modeling is the gas density. For five sources (W3, W3(OH), ρ Oph, W33, and Mon R2) we have strip maps of the CS $J = 2 \rightarrow 1$ 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_2O was computed using both the para- and ortho- H_2 collision rates with ortho- H_2O (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 ρ 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-H₂O abundance for the core, then computing the emission distribution, and finally convolving that distribution with the SWAS beam. The abundance of H₂O is varied until the modeled integrated intensity agrees with observations. We assume a constant H₂O abundance across each source. For positions with no detections, we used the 3σ upper limit on the integrated intensity to establish a 3σ upper limit on the H₂O abundance. The abundances and/or limits found for each core are given in Table 1. For S140 and ρ 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 H₂O 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-H₂O relative to H₂ varies from 6×10^{-10} to 1×10^{-8} . The highest H₂O abundances are derived for NGC 7538 and S140. The high H₂O 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_2O 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_2O found for the core center. The cloud core is extended to the north-east, and the absence of H_2O emission toward the positions east and north-east of the core center requires that either the abundance of ortho- H_2O 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_2O emission is most likely explained by a lower density and not a lower abundance. The non-detections of H_2O emission in the H₂O abundance reported in Table 1.

Although we believe that for most of the gas the H₂O 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 H₂O optical depth to scatter the line photons that arise from the core (Snell et al. 2000a). The H₂¹⁸O line should be less sensitive to these problems since it is optically thin, and therefore a more reliable estimator of the H₂O abundance. We have used the H₂¹⁸O observations toward the S140 core to establish an upper limit to the fractional abundance of ortho-H₂O. Using the same physical model described above, we derive a 3σ upper limit to the ortho-H₂¹⁸O abundance of 3×10^{-10} . As-

suming a ratio of H₂O/H₂¹⁸O of 500, this corresponds to a 3σ upper limit of 1×10^{-7} for the abundance of ortho-H₂O relative to H_2 . Comparing this result to our estimate of the H_2O abundance obtained from the more common isotopic species, it is not surprising that we were unable to detect $H_2^{18}O$ in this core.

We failed to detect H₂O emission from the three dark cloud cores observed by SWAS. Although we achieved similar signalto-noise ratio in all three cores, the higher density and column density in TMC-1 permit establishing a more stringent limit on the ortho-H₂O abundance. In TMC-1, we find a 3σ upper limit on the fractional abundance of ortho-H₂O of 7×10^{-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 H₂O 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-H₂O relative to H₂ in these cloud cores varies from 6×10^{-10} to 1×10^{-8} . The relative ortho-H₂O abundance in the majority of these cores is of order 1×10^{-9} , similar to the abundances found for M17SW (Snell et al. 2000b). In S140 the relative abundance of ortho-H₂O is about ten times larger, closer to the average ortho-H2O abundance for Orion (Snell et al. 2000a). In general the relative abundance of ortho-H₂O 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 μ m (van Dishoeck & Helmich 1996; Helmich et al. 1996; Gensheimer et al. 1996; van Dishoeck 1998). It it 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 μ m, 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 ≥300 K (van Dishoeck 1998; van Dishoeck et al. 1999). Abundance estimates for water in the hot cores range from 1×10^{-6} to 1×10^{-4} , several orders of magnitude greater than the abundance of water in the surrounding core gas. Even our limit on the H₂O abundance based on $H_2^{18}O$ in S140 rules out the possibility that the large H₂O abundance found for the warm gas applies to the general cloud core. At temperatures exceeding \sim 200-400 K, found in shocks and hot cores, a series of neutralneutral 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 H₂O 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 H₂O in the cold gas is even smaller than that quoted in Table 1.

Only upper limits to the ortho-H₂O 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-H₂O abundance is set in TMC-1, and in this core the 3σ upper limit on the H₂O 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 H₂O emission has been detected by SWAS toward two other class 0 protostellar cores, L1157 and NGC 1333 IRAS 4 (Neufeld et al. 2000). The H₂O emission in these sources clearly arises from the molecular outflows associated with class 0 sources. The relative abundance of ortho-H₂O in the outflow gas found by Neufeld et al. (2000) is of order 1×10^{-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 H₂O 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 H2O formation by neutral-neutral reactions is inhibited.

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