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A SEARCH FOR VIBRATIONALLY EXCITED H_2O AT 68 GHz

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ABSTRACT

Water vapor may be one of the most abundant constituents of shocked molecular clouds. The nonequilibrium distribution of population among its rotational energy states requires the observation of a multiplicity of transitions to constrain its abundance and excitation state. Flux limits are presented for emission due to the (010) $4_{14} \rightarrow 3_{21}$ rotational transition of ortho–H_2O at 67.804 GHz in several nebular and stellar sources. Upper limits for a beam-averaged column density of H_2O in its ν_2 vibrational manifold are derived for Orion BN-KL. Constraints placed by these observations on an internal source of infrared radiation in the Orion shock are discussed.

Subject headings: interstellar: molecules — line identifications — radio sources: lines

I. INTRODUCTION

A pivotal role is generally ascribed to water as a coolant in high-density molecular gas in standard models of both "J shocks" (Hollenbach and McKee 1989) and "C shocks" (Neufeld and Melnick 1987), but observational constraints on the physical conditions of water vapor in molecular shocks are lacking. Since the prevalence of 22 GHz maser emission indicates that water exists under conditions far from equilibrium, it is clear that a multiplicity of line observations are required to constrain those conditions. This is similarly true of the atmospheres of infrared stars which have been modeled in some detail (Deguchi 1977; Cooke and Elitzur 1985).

The presence of highly excited shocked molecular material suggests a search for water in its ν_2 (bending) mode, 1908 cm^{-1} above the ground state, as does the fact that various maser-excitation models invoke vibrational pumping. Emission lines connecting rotational levels of the vibrationally excited state are absorbed neither by the atmosphere nor by foreground cold H_2O in the source. While collisional pumping cannot account for appreciable abundances of vibrationally excited water, a mechanism may exist within the shock for significant IR excitation, such as that suggested by the Tarter and Welch (1986) model for grain heating and maser excitation within dense clumps. The infrared pumping model of Deguchi (1977) demonstrated that under some conditions of infrared pumping, such as in the atmospheres of IR stars, not only would the ν_2 excited state be populated, but appreciable inversions might obtain. In the subsequent Cooke and Elitzur (1985) model of H_2O excitation around late-type stars, the excited state was found to affect the population distribution among the ground state rotational levels at no more than the 10% level; however, population distribution within the excited state was not discussed. An earlier search for the (010) $4_{23} \rightarrow 3_{30}$ line of H_2O at 12.009 GHz (Myers and Barrett 1982) detected no emission in Orion at the 20 mK (1 σ) level. We have revisited this question by searching for the (010) $4_{14} \rightarrow 3_{21}$ line of H_2O at 67.804 GHz, the vibrationally excited analogue of the apparently masing 380 GHz line in the ground state. Subsequent searches at 96.261 and 232.687 GHz (Menten and Melnick 1989) have detected emission in the H_2O (010) mainfold in two stellar sources.

The 68 GHz line exhibits strong gain according to the IR excitation calculation of Deguchi (1977), and has a higher spontaneous transition probability than the 12 GHz line previously searched for, and thus more tightly constrains the abundance of H_2O in the vibrationally excited state. There are four dominant infrared transitions connecting each of the probed levels to the ground state. If we assume a ground state thermalized at a nominal 400 K, the temperature to which the gas is heated by H_2 formation in the postshock region where H_2O is primarily formed in the model of Hollenbach and McKee (1989), and further explore the implication of a continuum source of saturating 6.3 μm radiation, we find that pumping of the upper level is favored by 12%.

Water has been detected in star-forming regions in its ground state rotational transitions at 22, 183, 380, and 321 GHz (Menten, Melnick, and Phillips 1990) and in the isotopic variants, $H_2^{18}O$ at 203 GHz (Phillips *et al.* 1978; Jacq *et al.* 1988), and HDO, in which a total of 10 lines have been detected to date (Petuchowski and Bennett 1988; Jewell *et al.* 1989; Jacq *et al.* 1990). In Orion BN-KL, detected emission lines at 183 and 380 GHz include spectral features associated with the hot core, quiescent molecular ridge, and diffuse plateau components of the region (Frerking and Kuiper 1987). Even so, the role of H_2O in Orion and its associated outflow is still largely unknown. Kuiper *et al.* (1984*a*) offer a number of possible interpretations for a temporally coincident 22 GHz flare and 183 GHz line enhancement, the latter of which was accompanied by a shift in peak line frequency. Of the ground-state rotational transitions, only the 22 and 321 GHz lines have been detected in stars, with upper limits placed for the 183 GHz line in 14 late-type stars by Kuiper *et al.* (1984*b*).

Abundance: Shock models predict the liberation of water from grain mantles and the conversion to gaseous water of all oxygen not tied up in CO. These processes could account for water column densities as high as 10^{19} cm^{-2} (Elitzur, Hollenbach, and McKee 1989), suggesting that H_2O may be one of the most abundant molecules in molecular clouds. Assuming that half the cosmic abundance of oxygen is available to form H_2O (Draine and Roberge 1982), and that $n(CO)/n(H_2) \approx 8$–15×10^{-5}, the observations of hot rotationally (Watson *et al.* 1985) and vibrationally (Geballe and Garden 1987) excited CO suggest an H_2O column density in the postshocked gas of $(5$–$30) \times 10^{17}$ cm^{-2}. Knacke *et al.* (1988) have derived a column density limit of $N(H_2O) \leq 2.3 \times 10^{17}$ cm^{-2}, using infrared absorption, in a 20″ beam, against the BN infrared continuum. This limit assumes an excitation temperature of 150 K, and might be missing much of the shocked H_2O if it overlays the H_2 emission peaks ~30″ SE and ~18″ NNW of BN. Indeed, the warm component of CO emission detected by Boreiko and Betz (1989) extends between these peaks.

Shock Conditions: The high-velocity atomic and molecular emission detected in Orion BN-KL has been attributed to a dual shock driven by an outflow from the newly formed star, IRc2. In this picture, posited by Chernoff, Hollenbach, and McKee (1982), two shocks arise as the supersonic outflow impacts the interstellar medium: the "ambient shock" is a C-type shock which advances into the ISM, preceeded by a discontinuous J-type "wind shock," which abruptly decelerates the wind. Observations of H_2, CO, and OH have been modeled successfully by a continuous C-shock, with suggestions of a "warm," dense postshock region responsible for the observed vibrationally excited CO (Geballe and Garden 1987), as well as for the predominant contribution to the high J rotational CO emission (Boreiko and Betz 1989). While a continuous shock would be distinguished by an appreciable abundance of neutrals at $T > 1000$ K, rapid radiative de-excitation in the infrared might be expected to prevent polar molecules such as CO or H_2O from coming to collisional equilibrium with the surrounding gas. Some excited-state population, however, may be maintained radiatively if the cooling IR photons are unable to escape from the region. While the best-fit excitation temperture for the H_2 vibrational emission data is ~2200 K, Brand *et al.* (1988) have suggested that the data appear more characteristic of a cooling zone behind a hydrodynamic shock. Geballe and Garden (1987) have deduced that $v = 1$–0 CO line emission extends far into relatively cool postshock regions from the fact that the column density of hot CO of $\sim 2 \times 10^{18}$ cm^{-2} implies a column length of 2×10^{15} cm, compared to the column length of only 2×10^{13} cm inferred for vibrationally excited H_2.

The J-shock model of Hollenbach and McKee (1989) predicts that, while oxygen remains predominantly atomic, appreciable abundances of H_2O should be formed at a temperature plateau occurring at $T \sim 400$–500 K.

To further probe the physical state of the water constitutent of stellar and shock environments, we have observed four stars, selected on the basis of 22 GHz maser emission, and four regions of star formation similarly selected.

II. OBSERVATIONS AND ANALYSIS

Observations were made in 1988 April/May and 1988 October with the NRAO[1] 12 m telescope using the two-channel 3 mm Schottky receiver.

This is a double-sideband receiver, where the sidebands are separated by 3 GHz. Cold load Y-factor measurements gave system temperatures of 311 and 346 K for the two channels. The receiver back end consisted of two sets of filter banks in the "parallel" mode, where 128 channels of 1 MHz width each were run in parallel with 128 channels of 500 kHz each, with the same center frequency. The center frequency was chosen to be 67.780 GHz for the lower sideband and 70.780 GHz for the upper sideband, so that the $6_{15} \rightarrow 6_{06}$ $^{34}SO_2$ line at 67.768 GHz would fall within the same bandpass as the 67.804 GHz H_2O line. One day of each of the observing runs was spent at 2 MHz and 4 MHz frequency offsets to allow association of detected lines with respective sidebands.

Atmospheric opacity at this frequency is significant. It is dominated by O_2, and was measured in the following manner. Tipping scans were performed at two frequencies separated by 3 GHz, such that 67.8 GHz and 70.8 GHz fell sequentially in the lower sideband. The zenith atmospheric transmission measured at each of these frequencies corresponds to an average over the two sidebands, separated by 3 GHz, and each 600 MHz wide. By assuming a Lorentzian envelope for the O_2 manifold centered at 60 GHz, a zenith opacity of 0.54 ± 0.04 was determined for a 600 MHz passband centered at 67.8 GHz. The contribution of telluric H_2O to atmospheric opacity at zenith at that frequency is calculated to be less than 0.001. The H_2O line observations were restricted to air masses less than 2, where system temperatures were in the range of 1500–2000 K.

The beam size at 68 GHz was 1.′5, and thus encompassed the shocked molecular gas surrounding Orion BN. Pointing and focus corrections were made using Venus as a strong continuum source. The center beam position was $\alpha(1950.0) = 05^h32^m46.9^s$ and $\delta(1950.0) = -05°24′21″$. Double-beam switching, where the source was alternately placed in the signal beam and the reference beam with a commanded 4′ azimuth separation on the sky, was found to produce reasonable baselines despite the large atmospheric opacity.

A correction for source elevation was applied to individual spectra based on the assumption of a signal in the lower sideband. A quadratic baseline was removed from the average. The resulting spectrum, reflecting 514 minutes of integration on Orion, is shown in Figure 1, along with a shorter integration with the detection band shifted by 4 MHz. The resolution of the spectrum centered at 67.780 GHz is 1 MHz, while the shifted spectrum has been Hanning filtered. The rms noise levels in the unshifted and shifted spectra are 9.6 mK and 15.6 mK, respectively.

The $^{34}SO_2$ line at 67.768 GHz served as a system test line. Fitted as a simple Gaussian, it is centered at $v_{LSR} = 6.5$ km s^{-1}, and has a FWHM of 30.9 km s^{-1}. This is the first detection of the $6_{15} \rightarrow 6_{06}$ transition, whose upper level lies 22.4 K above the ground state. Scaling our beam-averaged state-specific column density to a beam size of 30″ to allow comparison with the 1.3 mm measurements by Blake *et al.* (1986), we derive $N(6_{15}) = 2.1 \times 10^{13}$ cm^{-2}. Our measurement agrees with the column density and rotational temperture derived by Blake *et al.* (1987), on the basis of which the SO_2 emission is attributed to the plateau region.

The $32_{5,27} \rightarrow 21_{6,26}$ line of vibrationally excited $^{32}SO_2$, at an excitation energy of 1300 K, is not present in our spectra at 70.771 GHz. A limit (3 σ) of $\int T\,dv < 0.29$ K km s^{-1} implies a column density, scaled to a beam size of 30″, of $N((010)\ 32_{5,27}) < 5.6 \times 10^{12}$ cm^{-2}, which is consistent with the data of Blake *et al.* (1987) for lower lying v_2 transitions.

A 3 σ limit of $\Delta T < 30$ mK can be placed on emission (or absorption) in Orion at the frequency of the H_2O (010) $4_{14} \rightarrow 3_{21}$ line at $v = 67.80396(10)$ GHz (Belov *et al.* 1987). The broad feature between 67.794 GHz and 67.801 GHz cannot confidently be identified as a line, nor can its sideband be identified since it falls below the noise in the shifted spectrum. Its frequency corresponds to no known line. No other features above 2 σ appear in any of the spectra with the exception of the spectrum of NGC 7538 plotted, in Figure 2, on an axis of v_{LSR}

[1] The National Radio Astronomy Observatory, NRAO, is operated by Associated Universities, Inc., under contract with the National Science Foundation.

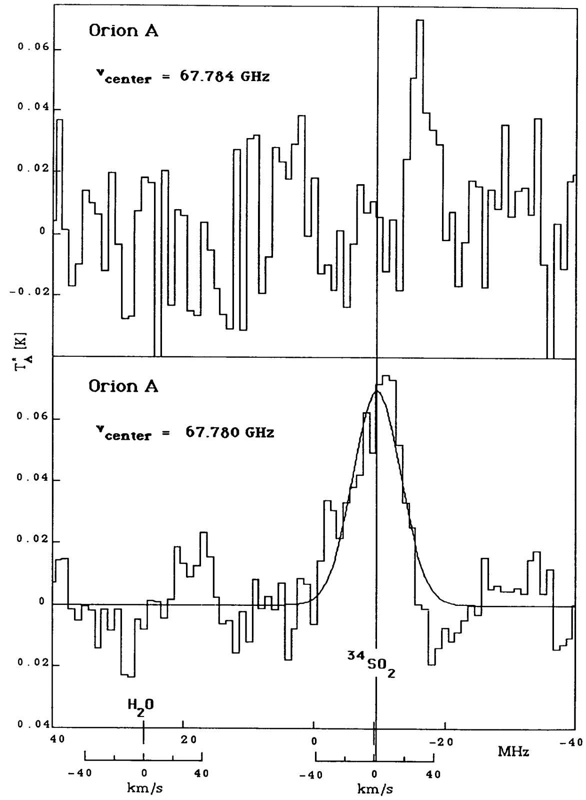

FIG. 1.—Observed spectra of Orion A, centered at 67.780 GHz (*lower*) and 67.784 GHz. The frequency resolution is 1 MHz per channel. The upper spectrum is Hanning filtered. Rest frequencies are shown for the $^{34}SO_2$ $6_{15} \rightarrow 6_{06}$ transition and the H_2O (010) $4_{14} \rightarrow 3_{21}$ line. A single Gaussian fit to the $^{34}SO_2$ line is shown.

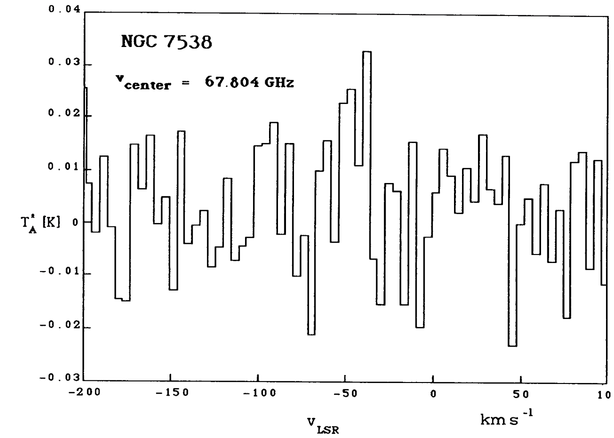

FIG. 2.—Observed spectrum of NGC 7538, based on 284 min integration on the source. The frequency resolution is 1 MHz per channel.

with respect to the rest frequency of the H_2O line. The peak of this spectrum is $< 3\ \sigma$, and lies well to the red of most maser features in NGC 7538 (Kameya *et al.* 1990). A high-velocity molecular flow component at -45–-40 km s^{-1} has been identified in CO spectra, however, by Kameya *et al.* (1989). Limits derived for other stellar and star-forming regions are given in Table 1.

III. DISCUSSION

Our flux density limits (less than 0.75 Jy, 3 σ) in the (010) $4_{14} \rightarrow 3_{21}$ line exclude optical gain lengths comparable to those of the 22 GHz ground state maser, in both shocked molecular and stellar environments. This allows for the expected spectral flux dilution, since we would expect lines in the stellar sources and individual features in the star-forming

TABLE 1

OBSERVED H_2O LINE FLUXES AND 1 σ RMS LIMITS

	(000)			(010)			
SOURCE	Peak S_{22} (Jy)	Max S_{183} (Jy)	Peak S_{321} (Jy)	Max S_{12} (Jy)	Max S_{68} (Jy)	Peak S_{96} (Jy)	Peak S_{232} (Jy)
Orion	4000[a]			<0.038[b]	< 0.23	<0.58[c]	<6.5[d]
Sgr B2	1000[a]					<1.2[c]	
W49	550[a]		140[e]	<0.034[b]	<0.30		
W3(OH)	4000[a]		140[e]	<0.027[b]	<0.33		
NGC 7538	700[a]			<0.027[b]	<0.25		
RX Boo	407[f]				<0.23	<0.2[g]	<0.25[h]
R Aql	237[f]	<2000[i]			<0.31		
RR Aql	353[f]	<2400[i]			<0.38		
OH 231.8+4.2	9[a]				<0.47		
VY CMa	$10^{(3-4)}$[j]		220[e]			16.7[g]	1.2[h]
W Hya	2000[f]					<0.07[g]	0.67[h]

[a] (1976/77 epoch) Genzel and Downes 1977 ($\Delta v = 0.43$ km s^{-1}).
[b] Myers and Barrett 1982 ($\Delta v = 1.5$ km s^{-1}).
[c] Turner 1989 ($\Delta v = 3.1$ km s^{-1}).
[d] Sutton *et al.* 1985 ($\Delta v = 1.3$ km s^{-1}).
[e] Menten *et al.* 1990 ($\Delta v = 0.46$ km s^{-1}).
[f] Spencer *et al.* 1979 ($\Delta v = 0.34$ km s^{-1}).
[g] Menton and Melnick 1989 ($\Delta v = 0.31$ km s^{-1}).
[h] Menton and Melnick 1989 ($\Delta v = 1.3$ km s^{-1}).
[i] Kuiper *et al.* 1984*b* ($\Delta v = 1$ km s^{-1}).
[j] (1969/76 epoch) Rosen *et al.* 1978 ($\Delta v = 0.14$ km s^{-1}).

regions not to be resolved. These observations are consistent with the negative results of Myers and Barrett (1982) in searching for the (010) 4_{23}–3_{30} transition of ortho-water.

A further limit, in Orion, is that set by the luminosity limit (3 σ) of 4.2×10^{41} photons s^{-1} for an unresolved isotropic source at $d = 480$ pc. Since the spontaneous emission probability of the 68 GHz line is $A = 2.3 \times 10^{-7}$ s^{-1}, the total number of H_2O molecules in the (010) 4_{14} state within the beam is $< 1.8 \times 10^{48}$ molecules. The implications of this limit are explored for the various regions within the beam.

a) The Extended Ridge Cloud

While an appreciable fraction of the flux at 183 GHz may be attributed to the "spike," or quiescent ridge (Waters *et al.* 1980; Frerking and Kuiper 1987), no source of IR flux is available to provide the vibrational excitation of the 68 GHz line. Comparing our beam-averaged column density limit of $N((010)\ 4_{14}) < 5.5 \times 10^{12}$ cm^{-2} with the total H_2O column density of 10^{17-18} cm^{-2} attributed by Waters *et al.* (1980) to this region, yields a fraction, $f((010)\ 4_{14}) < 10^{-4}$, consistent with expectations of negligible vibrationally excited water.

b) The Hot Core

For a radiatively dominated vibrational equilibrium, the ratio of vibrationally excited to ground state molecules (neglecting all higher lying modes) is

$$N(010)/N(000) = (\Omega/4\pi)(e^{h\nu/kT} - 1)^{-1} ,$$

where ν is the vibrational frequency, T is the radiation temperature of the excitation source, and Ω is the solid angle it subtends. Ziurys and Turner (1986) find their detection of vibrationally excited HCN consistent with location of the observed HCN in a clump on the wall of a cavity of radius 6–7 $\times 10^{16}$ cm surrounding the luminous IRc2 source, taken as a 700 K blackbody. Under these excitation conditions and assuming a distribution of H_2O among rotational levels reflecting a rotational temperature of 300 K (as characterizes the more highly excited species of the hot core, see Blake *et al.* 1987), the fractional population of the upper state of the interrogated transition would be $f((010)\ 4_{14}) = 1 \times 10^{-6}$. For an H_2 column of 1×10^{24} cm^{-2}, our limit of $N((010)\ 4_{14}) < 1.2 \times 10^{15}$ cm^{-2} $(6''/\theta)^2$ implies a fractional abundance $n(H_2O) = [H_2O]/[H_2] < 1 \times 10^{-3}$ $(6''/\theta)^2$, where θ is the angular extent of the emitting region. While this is similar to a limit derived from arguments based on the cosmic abundance of oxygen, it should be noted that *no* observation of which we are aware provides direct empirical evidence for the H_2O abundance of the hot core. A limit of $n(H_2O) < 2 \times 10^{-7}$, based on a search for H_2O^{18}, has been reported by Wannier *et al.* (1990). Chemical models (Graedel *et al.* 1982) suggest $10^{-6} < n(H_2O) < 10^{-5}$. Waters *et al.* (1980) and Frerking and Kuiper (1987) inferred an abundance, for the entire ridge cloud, of $n(H_2O) =$ 5–50 $\times 10^{-7}$. The nonthermal nature of the emission attributed to the hot core, however, does not allow abundances to be inferred. The evidence adduced by Jacq *et al.* (1988) for H_2O^{18} emission at a v_{LSR} characterizing the hot core is subject to varying interpretations. This should be borne in mind in drawing conclusions regarding isotopic fractionation effects when the abundance of HDO, clearly attributable to the hot core and compact ridge, is compared with an H_2O abundance which is either measured in a region characterized by substantially lower temperature or inferred from chemical models.

c) The High-Velocity Plateau and Shock

Kuiper *et al.* (1984*a*), detecting a broad emission feature at 183 GHz, argue that far-infrared radiation may pump the entire high-velocity plateau to emit in that transition. If we consider a radial scale of 10^{17} cm which corresponds both to the extent of the molecular plateau and to the maxima of vibrationally excited H_2, our search implies a column density limit of $N((010)\ 4_{14}) < \sim 6 \times 10^{13}$ cm^{-2}. We may assume that the partitioning of H_2O molecules among the states of the ν_2 manifold reflects rotational equilibrium among the ground state levels before vibrational excitation either by collision or radiative transition. At 400 K, this would put 4% in the 4_{14} state. Our observations, therefore, imply that no more than $\sim$0.2% of an assumed total H_2O column of $\sim 10^{18}$ cm^{-2} is vibrationally excited. If an internal source of infrared excitation such as dust establishes a population of vibrationally excited H_2O, then its temperature is limited by our observations to $<$400 K.

The higher kinetic temperature characteristic of a continuous shock would put a smaller fraction of the population into the 4_{14} state, and our limit would allow greater overall vibrational excitation, and a correspondingly higher limit on the temperature of any internal source of infrared radiation. For example, if the kinetic temperture of the neutral gas is 1000 K, then 1.6% of the vibrationally excited molecules would be in the 4_{14} state, placing an observational limit of 4×10^{15} cm^{-2} on the column of vibrationally excited H_2O molecules. The temperature of the grains, known to be only weakly coupled to the gas collisionally, must still be cooler than the gas or else the thickness of the region is significantly less than the mean free path for 6.3 μm radiation, since a 1000 K equilibrium abundance of vibrationally excited H_2O (11%) is excluded by our measurement.

d) The Postshock

Tarter and Welch (1986) invoke pumping of 22 GHz masers by infrared radiation diffusing into a clump of dense molecular material following its impact at a sufficiently high velocity with other dense material (perhaps a shell) in a molecular cloud. The essence of their scenario is the rapid diffusion into the clump of infrared radiation rising at the shock interface, giving rise to pumping of H_2O molecules out of the masing levels of the ground state at a differential rate. In the context of Orion, the Tarter and Welch (1986) model seeks to explain some 50 H_2O masers, each associated with a clump of radius 2–3 $\times 10^{14}$ cm. The total number of H_2O molecules represented by this matter is no more than 10^{51} $[n(H_2O)/10^5$ cm$^{-3}]$. Our observational limit of no more than 6% of this material in the (010) 4_{14} state places no real constraint on the viability of the model, since only $\sim$10% would be expected in the entire excited vibrational state, and less than 10^{-3} in the probed (010) 4_{14} state.

IV. SUMMARY

1. We place a flux limit (3 σ) of 0.75 Jy on emission (or absorption) in Orion A at the frequency of the H_2O (010) $4_{14} \rightarrow 3_{21}$ line at $\nu = 67.804$. Further observation of other water transitions is required to establish both the abundance and physical state of water giving rise to emission in the maser lines previously observed.

2. We have derived flux limits (3 σ) between 0.7 and 1.5 Jy in the (010) $4_{14} \rightarrow 3_{21}$ line of ortho–H_2O, in four stars and four

regions of star formation, all associated with H_2O maser emission.

3. Maser emission in the stellar environments, which might have been expected on the basis of the model of Deguchi (1977), is absent, suggesting that different classes of stellar H_2O masers might be distinguished by evidence of vibrationally excited population. This is true especially in light of positive detections by Menten and Melnick (1989). This suggests that more comprehensive models, including infrared pumping to higher lying vibrational manifolds, might be useful.

4. On the wing of the 60 GHz oxygen line, we have measured an atmospheric opacity of $\tau = 0.54 \pm 0.04$ in a 600 MHz bandwidth centered at 67.78 GHz.

5. A first detection of the 67.768 GHz $6_{15} \rightarrow 6_{06}$ transition of $^{34}SO_2$ in Orion is consistent with prior $^{34}SO_2$ measurements attributed to the high-velocity plateau.

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