1996ApJ...463L.109T

THE ASTROPHYSICAL JOURNAL, 463:L109–L112, 1996 June 1

POSSIBLE DISCOVERY OF THE 70 MICRON H_3O^+ $4_3^- \rightarrow 3_3^+$ TRANSITION IN ORION BN-IRc2

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Received 1996 January 17; accepted 1996 March 20

ABSTRACT

We report the first astronomical detection of a far-IR emission line at (69.524 ± 0.008) μm from aboard the Kuiper Airborne Observatory (KAO). We tentatively assign this line to the *R*-branch transition $4_3^- \rightarrow 3_3^+$ of H_3O^+. The wavelength of the discovered line lies between -112 and -60 km s^{-1} from predicted values. The position at which the emission line was detected is located about 20″ north of Orion BN, which is close to the shocked molecular hydrogen peak 1. We exclude hot shocked gas as the possible origin of the H_3O^+ emission. Hydrogen densities of $\gtrsim 5 \times 10^8$ cm^{-3} and temperatures $\gtrsim$100 K are required to match the observed integrated intensity of the 70 μm line. A speculative explanation for the 70 μm H_3^+O emission is that it might originate from very dense clumps.

Subject headings: ISM: abundances — ISM: clouds — ISM: individual (Orion BN-IRc2) — ISM: molecules

1. INTRODUCTION

Until very recently, only a few successful observations of water have been carried out in the Orion BN-IRc2 region, owing to strong telluric interference. In most of these cases this problem was circumvented by observations of isotopic water. Recent observations of the $H_2^{18}O$ 745 GHz $2_{11} \rightarrow 2_{02}$, 547 GHz $1_{10} \rightarrow 1_{01}$ (Zmuidzinas et al. 1995), and 184 μm $2_{21} \rightarrow 2_{12}$ (Timmermann et al. 1996) lines, however, could also not deduce the exact water abundance in Orion BN-IRc2, due to the notorious complexity of the region.

Since H_2O cannot be observed directly in many sources, an approach to estimate its abundance might be through observations of H_3O^+. H_2O forms directly from H_3O^+ through dissociative recombination with electrons (e.g., Phillips, van Dishoeck, & Keene 1992). However, it is clear that the H_2O abundance can be deduced reliably from that of H_3O^+ only if the chemistry is well known. Current models (Herbst & Leung 1989; Langer & Graedel 1989; Millar et al. 1991) predict $[H_2O]/[H_3O^+] = 500$–2000 and a fractional abundance $[H_3O^+]/[H_2] = (1$–$4) \times 10^{-9}$ for dense molecular clouds.

H_3O^+ has been observed through its $3_0^+ \rightarrow 2_0^-$, $1_1^- \rightarrow 2_1^-$, and $3_2^+ \rightarrow 2_2^-$, transitions at 396, 307, and 365 GHz, respectively, in Orion KL (Hollis et al. 1986; Wootten et al. 1986, 1991; Phillips et al. 1992). Figure 1 depicts the H_3O^+ energy level diagram. We note, however, most of these lines are confused by others such that their interpretation is not always certain. The H_3O^+ column densities that were derived for Orion KL ranged from 8×10^{13} to 7×10^{14} cm^{-2} corresponding to $[H_3O^+]/[H_2] = 3 \times 10^{-10}$–$3 \times 10^{-9}$.

Since the atmosphere at altitudes of 12.5 km is almost free of absorption for wavelengths around 69.5 μm, we have taken the opportunity to search for a transition in the *R* branch of H_3O^+ toward Orion BN-IRc2 from aboard the KAO. We have detected the first far-IR emission line at 69.524 μm, which we assign to the $4_3^- \rightarrow 3_3^+$ transition of H_3O^+. We note an alternative notation for this transition is *R*(3, 3).

2. OBSERVATIONS AND RESULTS

The observation of the H_3O^+ $4_3^- \rightarrow 3_3^+$ transition was carried out using NASA's KAO with the MPE/UCB Far-infrared Imaging Fabry-Perot Interferometer (FIFI). Full descriptions of the instrument are in Poglitsch et al. (1990, 1991) and Stacey et al. (1992). The beam shape on the sky was approximately Gaussian with a full width at half-maximum (FWHM) of about 24″ at 70 μm. The plate scale on the 5 × 5 element Ge:Ga detector array was 20″ $pixel^{-1}$. Observations were taken by chopping the telescope's secondary at 23 Hz. The chopper throw was 6′ in an approximately east-west direction. The pointing error is estimated to be $\lesssim$10″. The pointing accuracy was checked independently with the continuum flux distribution on the array. The observation of a point source, such as Orion BN, with a strong continuum provides a good test if the array moved on the sky during the observations and thus created artifacts in the spectra. In this case, one would see a sudden signal decrease in the pixels that showed a strong signal before and an increase of signal at other positions, while the high-order Fabry-Perot is scanning over the line of interest. However, no such an effect was detected. In our observations the array was centered on Orion BN which shows a continuum maximum (see 60 μm map of Thronson et al. 1986). The 70 μm H_3O^+ line emission was detected in the neighboring pixel just north of the center pixel, i.e., 20″ north of BN. Figure 2 shows the spectrum of the newly discovered line. All other elements of the array did not show any line emission at that wavelength. The data were obtained on a single flight at an altitude of 12.5 km on 1991 October 17. The spectral resolution was chosen to be 100 km s^{-1} (FWHM). The wavelength calibration was performed with a $D_2^{18}O$ absorption line at 69.5379 μm in the spectrometer's gas cell.

The line intensity was obtained by fitting a Lorentzian with a FWHM of 142 km s^{-1} superimposed on a flat continuum to

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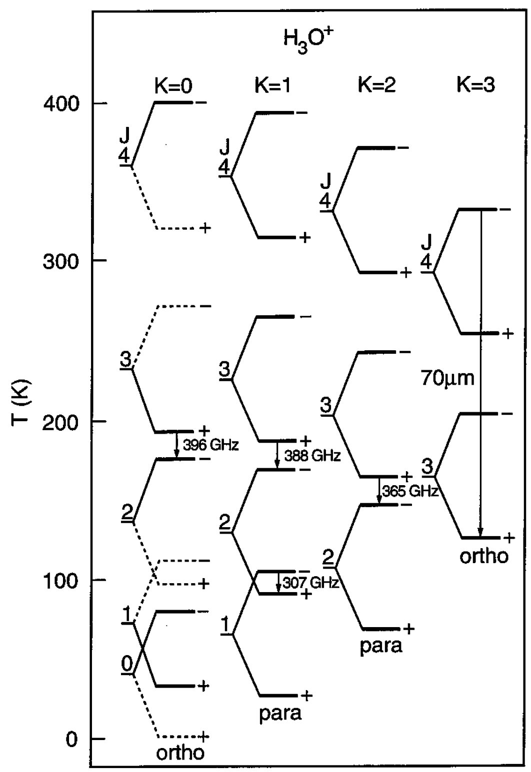

FIG. 1.—Energy level scheme of H_3O^+. The dashed lines indicate states with a statistical weight of 0. The submillimeter lines that have been observed previously (see text) are marked, as well as the $4_3^- \rightarrow 3_3^+$ transition at 69.524 µm. The 388 GHz line is accessible from ground-based telescopes but has not been observed yet.

the data. The relatively large width is surprising since no drifts in the calibration lines were detected. This would indicate an intrinsic line width of about 50 km s^{-1}. From the submm observations, we expect line widths $\lesssim 20$ km s^{-1}, so some additional velocity dispersion is indicated. Flat-fielding was achieved with internal hot and cold blackbody loads of known temperatures. The absolute intensity calibration was performed with measurements of the Orion KL region (Thronson et al. 1978). We estimate the absolute uncertainty of the line flux measurements to be about ±30%.

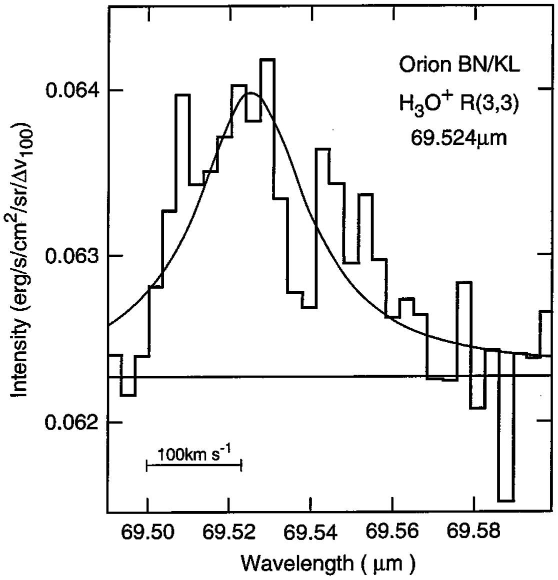

FIG. 2.—Spectrum of the H_3O^+ $4_3^- \rightarrow 3_3^+$ emission which was observed 20″ north of Orion BN. The FWHM of the fitted Lorentzian is 142 km s^{-1}.

We deduced a velocity integrated flux of $I_{70} = 5.1 \times 10^{-3}$ erg s^{-1} cm^{-2} sr^{-1} and a wavelength of (69.524 ± 0.008) µm for the emission line. We find that the observed line is shifted by −112 km s^{-1} with respect to the predicted wavelength of (69.55 ± 0.02) µm for the H_3O^+ $4_3^- \rightarrow 3_3^+$ transition (Liu & Oka 1985). The uncertainty corresponds to about 80 km s^{-1} (1 σ). In a later paper Liu, Oka, & Sears (1986) calculated a wavelength of 69.538 µm for this transition, corresponding to a shift of −60 km s^{-1}, however, no error is given for this wavelength. Since the wavelength of the observed line is within 1.5 σ from its predicted value, it is possible that it is the $4_3^- \rightarrow 3_3^+$ transition in H_3O^+. We note, however, that only a few high lying transitions in the R-branch of the $0^- \rightarrow 0^+$ band have been measured in the laboratory.

3. CALCULATIONS

3.1. *Model*

In order to obtain an estimate for the column density of H_3O^+ in Orion BN-IRc2, we solved the equations of statistical equilibrium and line formation for the states with $J \leq 4$ of ortho- and para-H_3O^+ (see also Fig. 1), which were treated as two separate species. Their energies were derived from molecular constants provided by Verhoeve et al. (1989). The highest level (4_0^-) lies at 365 K, the level of interest (4_3^-) lies at 305 K, above ground. Our model includes radiative transfer treated with an escape probability method. Stimulated absorption and emission was assumed through a background radiation field such that the gas sees 2π steradians of the dust continuum. The background source was Orion BN with a dust color temperature of $T_C = 72$ K. The radiation field is represented by an IR continuum of the form $I_\lambda^C = B_\lambda(T_C)$ $\{\tau_0 \times [60/\lambda(\mu m)]\}$, where B_λ is the Planck function and $\tau_0 = 0.503$ (Melnick et al. 1990). The statistical weights and radiative transition probabilities were calculated for a symmetric top molecule according to Townes & Schawlow (1955). For the calculation of the matrix elements, those with $\Delta J = 0, \pm 1$, $\Delta K = 0$, and $+ \leftrightarrow -$, we utilized the value for the electric Dipole moment of 1.438 debye computed from ab initio calculations for the $0^- \rightarrow 0^+$ band (Botschwina, Rosmus, & Reinsch 1983). Collisional transition rates for H_3O^+ with H_2 were adopted from Offer & van Hemert (1992) for the lowest five ortho- and seven para-states. The rates for the higher states were extrapolated from those of the lower states. As suggested by Phillips et al. (1992) collisional rates within one K-ladder are expected to scale with the radiative rates. For simplicity, we also took this approach to calculate the missing collision rates for the interladder transitions ($K = 0 \leftrightarrow 3$ and $1 \leftrightarrow 2$). It should be noted that the rates by Offer & van Hemert (1992) are uncertain by up to a factor of 5 (Phillips et al. 1992). Moreover, the collision rates for H_3O^+ are expected to also be different for different collision partners (ortho-H_2 or para-H_2). The ortho/para ratio of H_3O^+ was assumed to be unity which holds for temperatures $T \gtrsim 50$ K.

We point out that the excitation condition for the 70 µm $4_3^- \rightarrow 3_3^+$ transition is quite different from that of all previously observed submillimeter lines in the 300–400 GHz range. Due to the large Einstein coefficient ($A \approx 0.5$ s^{-1}) for the $4_3^- \rightarrow 3_3^+$ transition the critical density is $n_{\rm crit}(H_2) \approx 4 \times 10^{11}$

TABLE 1

Column Densities (cm^{-2}) of H_3O^+ Required to Match the Observed 70 micron Line Flux

$n(H_2)$ (cm^{-3})	T (K)			
	50	100	200	300
10^8	⋯	7.0E16	3.2E16	2.4E16
10^9	⋯	8.2E15	3.4E15	2.5E15
10^{10}............	2.0E16	1.1E15	4.4E14	3.2E14
10^{11}............	5.0E15	3.4E14	1.4E14	1.1E14
LTE	4.0E15	2.6E14	1.1E14	9.0E13

cm^{-3}, much higher than that [$n_{\rm crit}(H_2) \sim$ few $\times 10^6$ cm^{-3}] for the submillimeter lines.

3.2. *Results*

With the model described above we calculated the H_3O^+ column densities that are required to match the observed 70 μm line flux (see § 2). The results are presented in Table 1 for different gas temperatures and hydrogen densities (including an LTE case). The calculations assumed a beam filling factor of unity and a line width of $\Delta v = 30$ km s^{-1}. Unfortunately, we do not have independent H_3O^+ observations at the position 20″ north of BN to get tighter constraints on the parameters, such as temperature and density, because previous H_3O^+ observations were done on Orion KL, and the 396 GHz integrated line map (Phillips et al. 1992) does not extend that far north. However, we find that conditions of $n(H_2) \gtrsim 10^{10}$ cm^{-3} and $T \gtrsim 100$ K are required for the emitting gas if we simply assume that the H_3O^+ column densities for Orion KL and the position 20″ north of BN as inferred from the submillimeter line and 70 μm line, respectively, are of similar order [$N(H_3O^+) = 10^{14}$–10^{15} cm^{-2}]. This is due to the large critical density for the $4_3^- \rightarrow 3_3^+$ transition. We note also that hydrogen column densities $\gtrsim 10^{23}$ cm^{-2} are required for the emitting gas if we use theoretical fractional abundances (see § 1). Moreover, we have calculated the antenna temperatures for the 365 and 396 GHz lines for the position 20″ north of Orion BN that are shown in Table 2. The H_3O^+ column densities were adopted from Table 1. T_A scales with $N/\Delta v$. We note, however, that for hydrogen densities smaller than 10^9 cm^{-3} the submillimeter lines become optically thick, owing to the larger H_3O^+ column densities.

It is possible, however, that the estimated value for the critical density $n_{\rm crit}(H_2) = 4 \times 10^{11}$ cm^{-3} of the $4_3^- \rightarrow 3_3^+$ transition is too high, owing to uncertainties in the collision rate coefficients (see § 3.1). A conservative lower limit for the critical density can be deduced from observations of Orion KL. If we apply the derived parameters of Phillips et al. (1992) we find that the calculated line flux for the 70 μm line in Orion KL is too small to be detected. In fact, we definitely did not detect 70 μm line emission at that position. Only if the critical density was more than 20 times lower than the calculated value, we would have observed the 70 μm emission line. Therefore, this sets the lower limit to $n_{\rm crit}(H_2) \approx 2 \times 10^{10}$ cm^{-3} for the critical density. However, even if the critical density of the H_3O^+ $4_3^- \rightarrow 3_3^+$ line is 2×10^{10} cm^{-3}, the hydrogen density of the emitting gas still must be $n(H_2) \gtrsim 5 \times 10^8$ cm^{-3} to populate the 4_3^- level of H_3O^+ sufficiently.

TABLE 2

Calculated Antenna Temperatures T_A (K) for the H_3O^+ 365 and 396 GHz Lines

$n(H_2)$ (cm^{-3})	T (K)			
	50	100	200	300
10^8	⋯	69/134	59/163	50/126
10^9	⋯	15.5/38	8.2/19	6.3/15
10^{10}	18/29	2.4/5.5	1.1/2.9	0.82/2.3

Note.—The entry to the left of the slash is for the 365 and the entry to the right of the slash is for the 396 GHz line.

4. DISCUSSION

We have discovered a new emission line at (69.524 ± 0.008) μm, which we tentatively assign to the $4_3^- \rightarrow 3_3^+$ transition in the R-branch of H_3O^+. Since its wavelength is offset by about -60 km s^{-1} from the predicted value (Liu et al. 1986) we sought transitions in the JPL spectral line catalog (Poynter & Pickett 1985) that have similar wavelengths. These include several transitions in D_2O, HO_2, H_2O_2, and NH_2CN. None of these species turned out to be a likely candidate because their abundance in the ISM is thought to be too small or the states from which the transitions originate lie too high above their appropriate ground states. There is, however, one species, $HOCO^+$, which is a possible candidate for the emission line. $HOCO^+$ has two lines at 69.5235 ($23_{3\,21} \rightarrow 22_{2\,20}$) and 69.5192 μm ($23_{3\,20} \rightarrow 22_{2\,21}$). The transitions originate from states that lie about 615 K above the ground state. Unless the emitting gas is hot ($T > 500$ K) it is unlikely that these states are populated, particularly since the lower lying $HOCO^+$ $17_{11\,7} \rightarrow 16_{11\,6}$ and $17_{11\,6} \rightarrow 16_{11\,5}$ transitions at 362.012 and 364.803 GHz, respectively, are clearly not visible in the spectra of Phillips et al. (1992) and Wootten et al. (1991). In shocked gas such as the outflow from BN-IRc2 the situation might be different. We cannot entirely rule out this possibility, but again note that $HOCO^+$ has not been detected in the Orion KL region, even in transitions from low-lying states ($J \leq 5$) (Minh, Irvine, & Ziurys 1988).

The source of the 70 μm H_3O^+ emission is distinct from that of the submillimeter lines. It originates from a location 20″ north of Orion BN that is ≈5″ east of the shocked molecular hydrogen peak 1, whereas the submillimeter line emission is observed at the KL complex. Moreover, high values for the hydrogen densities of $\gtrsim 5 \times 10^8$ cm^{-3} are required to excite the upper level 4_3^- in order to match the observed 70 μm line flux. Following questions arise from the submillimeter and far-IR observations. Is there any reason to believe there are two distinct positions of H_3O^+ emission? Is there a region in BN-IRc2 with very high densities? Does the 70 μm line originate from shocked gas?

Calculations with a C-shock model (Timmermann 1996) indicate that shocks of this type are no good candidates to explain the observed 70 μm line because the integrated H_3O^+ column density across the region of hot shocked gas turns out to be only $N \sim 10^9$ cm^{-2}. We note that also fast shocks of J-type (see Neufeld & Dalgarno 1989) fail by far to produce the observed H_3O^+ column densities. Furthermore, the density of molecular hydrogen in the shocked gas around Orion BN-IRc2 is only of order 10^6 cm^{-3} as commonly inferred from C-shock models. Another possible origin of the 70 μm emission is postshocked gas with densities of $\approx 10^7$ cm^{-3}. It seems, however, that even this value is not adequate to populate the 4_3^- level of H_3O^+, particularly since the expected temperature

$T < 100$ K in postshocked gas is too low along with the estimated column density of hydrogen $N(H_2) \approx 10^{22}$ cm^{-2}.

We can also exclude that the 70 μm emission originates from the "hot core" in the Orion KL complex owing to the positional offset and its small size of ≈10″. Furthermore, the molecular hydrogen density in the "hot core" is of order a few $\times 10^7$ cm^{-3} (Genzel & Stutzki 1989). The Orion "plateau" region, however, is much more extended as seen from water vapor observations at 183 GHz (Cernicharo et al. 1994). The high-velocity plateau emission seems to extend as far as ≈40″ from IRc2 and has an elongated shape in an north-south direction. If, according to interstellar chemistry models, the H_3O^+ density is linked to that of H_2O one would expect also extended H_3O^+ emission. Again we note that the size of the 70 μm emitting region is definitely not larger than about 20″ and also offset with respect to the KL complex. Furthermore, the gas density in the Orion "plateau" is even lower than in the "hot core."

If the H_3O^+ emission originates from two distinct peaks, i.e., H_2 peak 1 and Orion KL, the density at peak 1 must be higher than at KL because the 70 μm emission line is observed at peak 1 only owing to the higher critical density compared to those of the submillimeter lines. Currently available observations of other species, however, do *not* provide any evidence for a higher density at peak 1. Furthermore, it seems that the submillimeter lines should be also detectable at peak 1 as well, since according to the calculations (see Table 2 and § 3.2) the 365 and 396 GHz lines are fairly strong for $n(H_2) < 10^{10}$ cm^{-3}, provided of course the rate coefficients are correct.

The entire region of BN-IRc2 is notoriously complex. Therefore, it is possible but speculative that dense, high-velocity clumps in the outflow from BN-IRc2 might be the origin of the 70 μm H_3O^+ emission. These clumps are commonly observed through masing transitions such as those of H_2O and SiO and are known to have densities of order 10^9 cm^{-3} and temperatures greater than 100 K, sufficient to excite the 4_3^- level of H_3O^+. However, the size of these clumps is $\sim 3 \times 10^{13}$ cm so that the beam-filling factor is probably small. In addition, the inferred hydrogen column density is of order $\sim 3 \times 10^{22}$ cm^{-2}. If we apply the theoretical fractional abundance (see § 1) we get $N(H_3O^+) \sim 10^{14}$ cm^{-2}, which is about similar to the values derived for Orion KL. It is possible, however, that in such hot, dense clumps the abundance of H_3O^+ might be higher instead. But this assumption needs to be checked with the appropriate oxygen chemistry. The question of the presence of high-density gas in the shocked region peak 1 of Orion BN-IRc2 might be answered through observations of high-density tracers such as relatively high-lying transitions of HCN, CS, or H_2CO. We also expect that ISO will detect many more transitions, possibly those in the *R* branch of H_3O^+ in various astronomical sources and may help to solve this apparent problem.

We are grateful to the staff of the KAO for their competent support. We thank Suzanne Madden for helping with the observations and Ewine van Dishoeck, Malcolm Walmsley, and Chris Wright for fruitful discussions. This work was partially supported by NASA grant NAG-2-208 to the University of California, Berkeley. N. G. was supported by a Feodor Lynen fellowship of the Alexander von Humboldt foundation.

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