K-band Radio Observations of Comet Hale-Bopp: Detections of Ammonia and (Possibly) Water

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Abstract. K-band radio observations of comet Hale-Bopp (C/1995 O1) were conducted in March/April 1997 at the 100-m Telescope of the Max-Planck-Institut für Radioastronomie. Emission was firmly detected from the five lowest metastable (J=K) inversion transitions of ammonia. Assuming a thermal distribution for the metastable states of NH_3, we derive a rotational temperature of 104±30 K and an ammonia production rate at perihelion of $6.6\pm1.3 \times 10^{28}$ s^{-1}. The updated ammonia-to-water abundance ratio is found to be of the order of 1.0%. We also report a marginal detection of the 6_{16}–5_{23} transition line of water at $\lambda = 1.35$ cm.

Key words: radio line emission, comets, comet Hale-Bopp

1. Introduction

Radio emission from ammonia was detected in the gas coma of comet Hale-Bopp (C/1995 O1) at the 100-m Radio Telescope of the Max-Planck-Institut für Radioastronomie (MPIfR) in Effelsberg, Germany. Line profiles of all NH_3 inversion transitions in the metastable states (J=K) up to (J,K) = (5,5) were observed in March/April 1997. The 6_{16}–5_{23} transition line of water at $\lambda = 1.35$ cm was marginally detected during the same observation epoch. A summary of the results for ammonia was published by Bird *et al.* (1997).

Ammonia was first successfully detected at MPIfR by Altenhoff *et al.* (1983) in comet IRAS-Araki-Alcock (1983d = 1983 VII). Palmer *et al.* (1996) reported detections of both the (1,1) and (3,3) lines in comet Hyakutake (C/1996 B2) at the NRAO 43-m Green Bank telescope. Both of these detections occurred at unusually close Earth range ($\Delta \sim 0.04$ and 0.10 AU, respectively). Many unsuccessful searches for

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ammonia and/or water have been conducted previously at MPIfR (e.g., Bird *et al.*, 1997; and references therein).

2. Observations

Ammonia was observed at MPIfR on four 1997 days: 13,25 March, and 1,3 April. A tabular summary and additional technical details of the observations, as well as a figure showing the averaged spectra over all observation days, may be found in Bird *et al.* (1997).

For optically thin emission the beam-averaged column density in both the upper and lower level of the specific NH_3 state is given in cgs units by (e.g., Rohlfs and Wilson, 1996):

$$\langle N(J,J)\rangle = 6.8 \times 10^{12} \; \frac{J+1}{J} \int T_{MB}(v) \; dv \quad [\mathrm{cm}^{-2}] \tag{1}$$

for T_{MB} in K and the velocity scale dv in km s^{-1}. The integrated line strength was computed from $\int T_{MB}\, dv \simeq 1.064 \cdot T_{peak} \cdot \delta v$.

Assuming thermal equilibrium in the comet's inner coma, the relative populations of the lowest metastable states will depend on the "rotational temperature" T_R, which should be representative of the neutral gas temperature. Having derived the beam-averaged column densities according to Eq. (1), Bird *et al.* (1997) constructed a "Boltzmann Diagram", a log-log plot of $\langle N(J,J)\rangle/[g_{op}(K)(2J+1)]$ vs. energy W(J=K) of each state above ground, to estimate T_R. The factor $g_{op}(K)$ is 2 for K = 0,3,6,... (ortho-NH_3) and 1 for K = 1,2,4,5,... (para-NH_3). A least-squares best fit to the data yields T_R = 104±30 K, a temperature applicable to the region bounded by the extent of the NH_3 cloud.

The average spectrum of comet Hale-Bopp at the frequency of the water 6_{16}–5_{23} transition (ν = 22.235 GHz) is shown in Fig. 1. The full-range spectrum (upper panel) was obtained on 25 March (24 minutes on-source) and 1 April (39 minutes on-source). A Gaussian least-squares fit to the spectrum (lower panel) yields a marginal detection with $T_{peak} \simeq 58$ mK (1.7 σ) centered very near the velocity of the comet ($v_0 \simeq$ -0.13 km s^{-1}). The full linewidth was $\delta v \simeq 2.5$ km s^{-1}.

Again assuming the radio emission to be optically thin, an estimate of the water column density in the 5_{23} level may be obtained from (e.g., Rohlfs and Wilson, 1996):

$$\langle N(5_{23})\rangle = 2.07 \times 10^{3} \frac{g_l \nu^2}{g_u A_{ul}} \int T_{MB}\; dv \quad [\mathrm{cm}^{-2}] \tag{2}$$

where ν = 22.235 GHz, $A_{ul} = 1.91 \times 10^{-9}$ s^{-1} is the Einstein coefficient, and g_l, g_u are g-factors for the lower and upper levels of the transition,

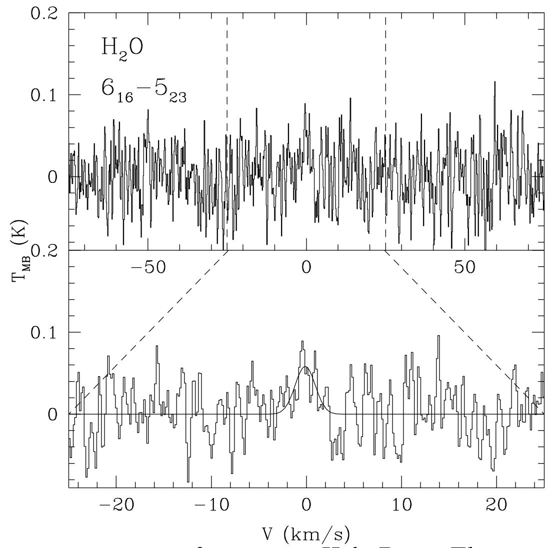

Figure 1. Mean water spectrum from comet Hale-Bopp. The upper panel shows the complete bandpass and the lower panel shows the spectrum at higher resolution with the Gaussian line fit (T_{peak} = 58±13, v_0 = -0.13±0.27, $FWHM = \delta v$ = 2.49±0.64).

respectively. Eq. (2) yields $\langle N(5_{23})\rangle = 6.8 \pm 1.4 \times 10^{13}$ cm^{-2} for the line strength derived from the H_2O detection in Fig. 1.

As a reference estimate, we can calculate the total water column density in the telescope beam under the assumptions that: (1) the water line is emitted under LTE conditions, (2) all H_2O levels in the cometary coma are populated thermally, and (3) the rotational temperature is $T_R = 104 \pm 30$ K as derived from the ammonia observations. Under these conditions, we can apply the following formula for the 5_{23} state (Rohlfs and Wilson, 1996):

$$\langle N(H_2O)\rangle = \langle N(5_{23})\rangle \frac{Z}{(2J+1)\; g_{op}(Ka,Kc)} \exp\left[\frac{W(5_{23})}{kT_R}\right] \qquad (3)$$

where the total partition function Z, appropriately accounting for the two identical H nuclei, is given in cgs units by:

$$Z = 337.4\sqrt{T_R^3/ABC} \qquad (4)$$

with A = 835.8 GHz, B = 435.4 GHz, C = 278.1 GHz the rotational constants for H_2O. The spin statistical weight in Eq. (3) with (J,Ka,Kc) = (5,2,3) is $g_{op}(2,3) = 3$ (ortho H_2O), and $W(5_{23})/k$ = 642.9 K. The total beam averaged H_2O column density computed from Eq. (3) with T_R = 104 K is $\langle N(H_2O)\rangle \simeq 521\ \langle N(5_{23})\rangle \simeq 3.6 \times 10^{16}$ cm^{-2}. Only about 0.2% of the H_2O molecules are in the 5_{23} (or 6_{16}) states. Radiative decay in the outer coma should depopulate these levels below their LTE values (Bockelée-Morvan, 1987). The detection of the $\lambda = 1.35$ cm emission line would thus imply an even higher value of $\langle N(H_2O)\rangle$ from Eq. (3).

Whereas the NH_3 column density was rather insensitive to the assumed excitation temperature, the situation is quite different for H_2O. If the excitation temperature is at the lower end of the range determined from the ammonia observations ($T_R = 74$ K), the H_2O column density computed from Eq. (3) increases by more than a factor of 7. Considering the much larger size of the water coma and the trend to higher temperatures at cometocentric distances $R > 5000$ km, a more appropriate value might be closer to the upper end of the temperature range from the ammonia observations ($T_R \simeq 134$ K). The water column density from Eq. (3) decreases in this case to a more plausible value of $\langle N(H_2O)\rangle \simeq 1.3 \times 10^{16}$ cm^{-2}.

3. Estimates of the comet's production rate

The production rate can be calculated from the observed column density if assumptions are made about the outflow velocity and lifetime of the specific molecule. After sublimation from the comet's nucleus, the parent molecules are destroyed by photo-dissociation/-ionization, gas chemistry, etc. For both water and ammonia, the source of the emission was centered on the velocity of the nucleus to within the measurement error. For optically thin emission, the linewidth δv is given by twice the outflow velocity $u = \delta v/2 \simeq 0.7$–$1.25$ km s^{-1}.

The lifetime of the ammonia molecule, which probably lies in the range 5.35×10^3 s $< \tau_a < 5.88\times10^3$ s depending on solar activity (Huebner *et al.*, 1992), is short enough that the emission region is much smaller than the MPIfR telescope beam for these observations. In this case (unresolved source), the beam-averaged column density $\langle N(NH_3)\rangle$ is related to the production rate $Q(NH_3)$ by (e.g., Snyder, 1982):

$$\langle N(NH_3)\rangle = \frac{4Q(NH_3)}{\pi\delta v\ d}\left[\frac{d}{\Delta\theta}\right]^2 = \frac{4Q(NH_3)\tau_a r^2}{\pi\Delta^2\theta^2}, \qquad d << \Delta\theta \quad (5)$$

where $d = \delta v \cdot \tau_a \cdot r^2$ is the diameter of the source region (r in AU), Δ is distance from Earth, and θ is the $HPBW$ of the antenna. Using $\theta \simeq 42''$ and $\tau_a = 5600$ s, the mean values of d and $\Delta\theta$ during the 4 observation days were 9.9×10^3 km and 40×10^3 km, respectively. Normalized to the perihelion date, Bird *et al.* (1997) obtained $Q(NH_3) = 6.6\pm1.3 \times 10^{28}$ s^{-1} ($\sim$2 tons per second) from Eq. (5).

Evidence for temporal variability is reflected in the spectra of the (3,3) line for each day (Fig. 2). The NH_3 column density from Eq. (1), and the production rates from Eq. (5) are presented in Table I. The

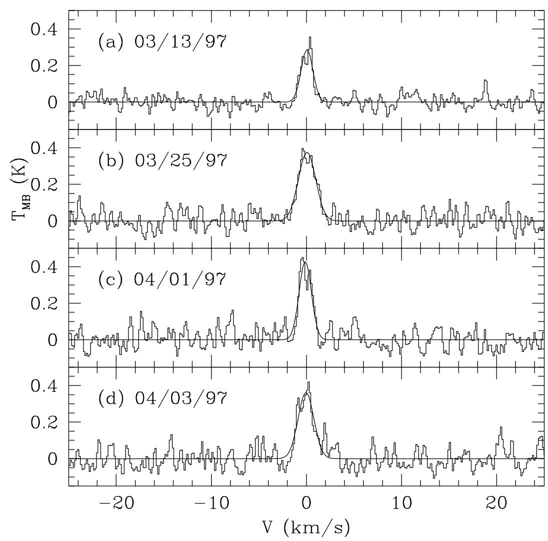

Figure 2. NH_3 (3,3) spectra from comet Hale-Bopp during the 4 observation days.

Table I. Ammonia (3,3) spectral line data for each observation date

date	T_{peak} [mK]	v_0 [km s^{-1}]	$FWHM = \delta v$ [km s^{-1}]	$\langle N(3,3) \rangle$ [10^{12} cm^{-2}]	Q(NH_3) [10^{28} s^{-1}]
13.26 Mar	287±16	0.06±0.04	1.47±0.10	4.4±0.9	3.3±0.7
25.31 Mar	375±17	0.07±0.05	2.15±0.11	8.5±1.7	6.7±1.3
01.34 Apr	426±22	-0.12±0.04	1.54±0.09	6.9±1.4	5.9±1.2
03.31 Apr	361±20	-0.04±0.05	1.96±0.13	7.4±1.5	6.5±1.3

line was strongest in the second observation session (between closest approach to Earth and perihelion). The ammonia production rate $Q(NH_3)$ is plotted in the upper panel of Fig. 3 for the four observation days. The middle and lower panels shows the corresponding peak main beam temperature T_{peak} and the linewidth δv, respectively. The solid horizontal lines in Fig. 3 denote the mean value over the four observations; the error bars at the far right indicate the rms deviation $\pm\sigma$ about the mean. The linewidth variations, rather than the peak temperature, tend to drive the variations in production rate.

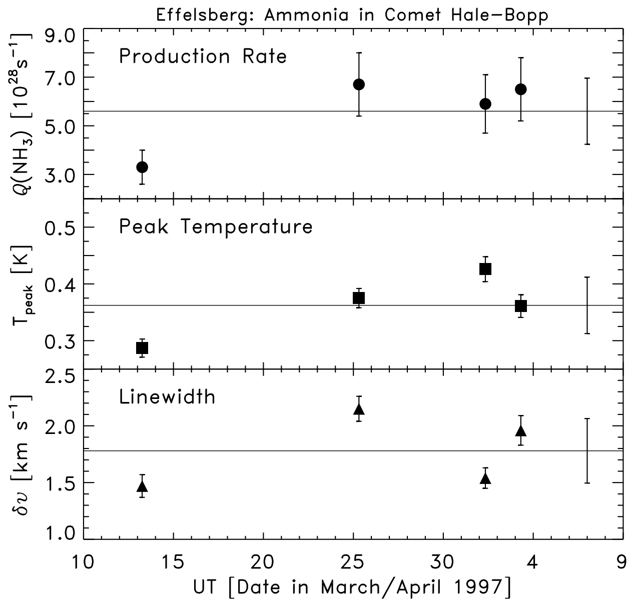

Figure 3. Variations in NH_3 production rate (upper panel), peak antenna temperature (middle panel) and linewidth (lower panel) in C/Hale-Bopp near perihelion. The horizontal lines are the mean value of the four measurements; error bars at right indicate ± the standard deviation.

In contrast to ammonia, cometary water emission is an intricate combination of collisional excitation, IR pumping, rotational decay and optical depth effects (Bockelée-Morvan, 1987). Thermal excitation of the 6_{16}–5_{23} transition is severely inhibited in the relatively cool coma. Indeed, the MPIfR detection of H_2O with $T_{peak} \simeq 58$ mK (Fig. 1) is quite marginal. Nonetheless, because C/Hale-Bopp is such an extraordinary object, it is still instructive to compute the H_2O production based solely on the basis of thermal excitation for comparison with estimates from other observers.

The lifetime for water at 1 AU (Huebner *et al.*, 1992) ranges from $\tau_w \simeq 5.7 \times 10^4$ s (active sun) to $\tau_w \simeq 9.7 \times 10^4$ s (quiet sun). Using an intermediate value $\tau_w \simeq 8.4 \times 10^4$ s, and an expansion velocity inferred from the observation $u = \delta v/2 \simeq 1.25$ km s^{-1}, the diameter of the potential source region of water emission is $d = \delta v \cdot \tau_w \cdot r^2 \simeq 1.8 \times 10^5$ km. Because this region subtends a much larger area than the telescope beam (resolved source), the beam-averaged column density is, to first order, independent of the size of the source d. In this case we obtain

$$\langle N(H_2O) \rangle = \frac{2Q(H_2O)}{\delta v \; \Delta\theta}, \quad d >> \Delta\theta \tag{6}$$

Using the column density $\langle N(H_2O)\rangle \simeq 1.3 \times 10^{16}$ cm^{-2} derived in the previous section, Eq. (6) yields a production rate of $Q(H_2O) \simeq 7 \times 10^{30}$ s^{-1}. The actual production rate is likely to be higher because, for a given column density, the circular aperture approximation in Eq. (6) will underestimate the production rate with respect to a more precise calculation using a Gaussian beam.

4. Discussion

Observations of comet Hale-Bopp by Biver *et al.* (1997; 1998) have shown that significant variations in the abundances of the coma constiuents occur within the same apparition, possibly due to varying sublimation energies and/or exposure of different surface areas from the changing aspect of the comet's rotation axis.

The MPIfR radio observations of NH_3 in comet Hale-Bopp near its perihelion have been used to derive a production rate of $Q(NH_3) \simeq 6.6 \times 10^{28}$ s^{-1} and a probable kinetic temperature of the inner coma ($R < 5000$ km) of $T_R \simeq 104$ K. The ammonia-to-water abundance ratio published by Bird *et al.* (1997), based on preliminary estimates of the water production rate at perihelion, was 1.4±0.4%.

More recent estimates of $Q(H_2O)$ have now been provided by various groups. The IR data have remained close to the original estimate of $Q(H_2O) \simeq 0.5 \times 10^{31}$ (e.g., Dello Russo *et al.*, 1998) but radio observations of OH tend to yield higher values of $Q(H_2O) \simeq 1.0 \times 10^{31}$ (Colom *et al.*, 1998). Evidence was presented by Biver *et al.* (1998) for enhanced outgassing of many molecular species near perihelion, thereby implying a value of $Q(H_2O)$ in the upper part of the probable range. Should this higher estimate be correct, the NH_3 abundance would have to be revised downward to about 0.7% and its ranking in the hierarchy of cometary nucleus constituents would probably fall a few notches. The NH_3 production rate is thought to be accurate to about 20% (Bird *et al.*, 1997). The uncertainty in the ammonia-to-water abundance is thus dominated by the relatively large error (factor of 2) associated with the H_2O production rate.

Relative NH_3 abundances have been estimated to be 0.1–0.2% from optical NH_2 spectra (Wyckoff *et al.*, 1991) and 0.44–0.94% from UV spectra of the NH radical (Feldman *et al.*, 1993), assuming that the observed species were dissociation products. An ammonia production rate of $1.5^{+0.5}_{-0.7}$% relative to water was derived for comet P/Halley (Meier *et al.*, 1994) from Giotto mass spectrometer measurements.

An ammonia abundance of 0.3% was derived from radio observations for C/Hyakutake by Palmer *et al.* (1996), considerably less than the corresponding abundance estimate for comet IRAS-Alraki-Alcock of 6% (Altenhoff *et al.*, 1983). Both of these values should be revised in the light of better $Q(H_2O)$ estimates that have been published in the interim. Using $Q(H_2O) = 1.7 \times 10^{29}$ for C/Hyakutake on the day of the NH_3 observations (Mumma *et al.*, 1996), the relative ammonia abundance for that comet increases to 0.6%. Feldman *et al.* (1984) derive $Q(H_2O) = 3.3 \times 10^{28}$ for comet IRAS-Alraki-Alcock from IUE observations performed on the same day as the Effelsberg observations, decreasing the relative NH_3 abundance down to a more reasonable value of 1.8%. The general trend of all previous radio detections of NH_3, including that reported for C/Hale-Bopp in this work, thus seems to be headed toward an relative abundance near or slightly below 1%.

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