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 NH₃, we derive a rotational temperature of 104±30 K and an ammonia production rate at perihelion of 6.6±1.3 × 10²⁸ 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 λ = 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 NH₃ 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 λ = 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 (Δ ~ 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., Rohlfis and Wilson, 1996):

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

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 $K = 0, 3, 6, \ldots$ (ortho-NH$_3$) and 1 for $K = 1, 2, 4, 5, \ldots$ (para-NH$_3$). A least-squares best fit to the data yields $T_R = 104 \pm 30$ 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 $6_1-5_{23}$ transition ($\nu = 22.235$ 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 $\sigma$) 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., Rohlfis and Wilson, 1996):

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

where $\nu = 22.235$ 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 ($T_{peak} = 58\pm13$, $v_0 = -0.13\pm0.27$, FWHM = $\delta v = 2.49\pm0.64$).

respectively. Eq. (2) yields $\langle N(5_{23}) \rangle = 6.8\pm1.4 \times 10^{13}$ cm$^{-2}$ for the line strength derived from the H$_2$O 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$_2$O levels in the cometary coma are populated thermally, and (3) the rotational temperature is $T_R = 104\pm30$ K as derived from the ammonia observations. Under these conditions, we can apply the following formula for the $5_{23}$ state (Rohlf and Wilson, 1996):

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

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

$$Z = 337.4 \sqrt[3]{T_R^3/ABC}$$  \hspace{1cm} (4)

with $A = 835.8$ GHz, $B = 435.4$ GHz, $C = 278.1$ GHz the rotational constants for H$_2$O. The spin statistical weight in Eq. (3) with $(J, Ka, Kc) = (5,2,3)$ is $g_{op}(2,3) = 3$ (ortho H$_2$O), and $W(5_{23})/k = 642.9$ K. The total beam averaged H$_2$O column density computed from Eq. (3) with $T_R = 104$ K is $\langle N(H_2O) \rangle \approx 521 \langle N(5_{23}) \rangle \approx 3.6 \times 10^{16}$ cm$^{-2}$. Only about 0.2% of
the H$_2$O 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$_2$O. If the excitation temperature is at the lower end of the range determined from the ammonia observations ($T_R = 74$ K), the H$_2$O 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 $\delta v$ is given by twice the outflow velocity $u = \delta v / 2 \approx 0.7$–1.25 km s$^{-1}$.

The lifetime of the ammonia molecule, which probably lies in the range $5.35 \times 10^3$ s $< \tau_a < 5.88 \times 10^3$ s depending on solar activity (Huebner et al., 1992), is short enough that the emission region is much smaller than the MPIIR 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):

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

where $d = \delta v \cdot \tau_a \cdot r^2$ is the diameter of the source region ($r$ in AU), $\Delta$ is distance from Earth, and $\theta$ is the HPBW of the antenna. Using $\theta \approx 42''$ and $\tau_a = 5600$ s, the mean values of $d$ and $\Delta \theta$ during the 4 observation days were $9.9 \times 10^3$ km and $40 \times 10^3$ km, respectively. Normalized to the perihelion date, Bird et al. (1997) obtained $Q(NH_3) = 6.6 \pm 1.3 \times 10^{28}$ s$^{-1}$ (~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

![Image](image_url)

*Figure 2. NH$_3$ (3,3) spectra from comet Hale-Bopp during the 4 observation days.*

<table>
<thead>
<tr>
<th>date</th>
<th>$T_{peak}$ [mK]</th>
<th>$v_0$ [km s$^{-1}$]</th>
<th>FWHM = $\delta v$ [km s$^{-1}$]</th>
<th>$\langle N(3,3) \rangle$ [$10^{12}$ cm$^{-2}$]</th>
<th>Q(NH$_3$) [$10^{26}$ s$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>13.26 Mar</td>
<td>287±16</td>
<td>0.06±0.04</td>
<td>1.47±0.10</td>
<td>4.4±0.9</td>
<td>3.3±0.7</td>
</tr>
<tr>
<td>25.31 Mar</td>
<td>375±17</td>
<td>0.07±0.05</td>
<td>2.15±0.11</td>
<td>8.5±1.7</td>
<td>6.7±1.3</td>
</tr>
<tr>
<td>01.34 Apr</td>
<td>426±22</td>
<td>-0.12±0.04</td>
<td>1.54±0.09</td>
<td>6.9±1.4</td>
<td>5.9±1.2</td>
</tr>
<tr>
<td>03.31 Apr</td>
<td>361±20</td>
<td>-0.04±0.05</td>
<td>1.96±0.13</td>
<td>7.4±1.5</td>
<td>6.5±1.3</td>
</tr>
</tbody>
</table>

The 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 $\delta v$, 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 ±σ about the mean. The linewidth variations, rather than the peak temperature, tend to drive the variations in production rate.
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 MPIIR detection of H$_2$O with $T_{\text{peak}} \approx 58$ mK (Fig. 1) is quite marginal. Nonetheless, because C/Hale-Bopp is such an extraordinary object, it is still instructive to compute the H$_2$O 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 $\tau_w \approx 5.7 \times 10^4$ s (active sun) to $\tau_w \approx 9.7 \times 10^4$ s (quiet sun). Using an intermediate value $\tau_w \approx 8.4 \times 10^4$ s, and an expansion velocity inferred from the observation $u = \delta v / 2 \approx 1.25$ km s$^{-1}$, the diameter of the potential source region of water emission is $d = \delta v \cdot \tau_w \cdot \tau^2 \approx 1.8 \times 10^3$ 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

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

(6)
Using the column density $\langle N(H_2O) \rangle \simeq 1.3 \times 10^{16} \text{ cm}^{-2}$ derived in the previous section, Eq. (6) yields a production rate of $Q(H_2O) \simeq 7 \times 10^{30} \text{ s}^{-1}$. 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 constituents 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 $Q(NH_3) \simeq 6.6 \times 10^{28} \text{ s}^{-1}$ and a probable kinetic temperature of the inner coma ($R < 5000 \text{ km}$) of $T_K \simeq 104 \text{ K}$. 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 $Q(H_2O) \simeq 0.5 \times 10^{33}$ (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$_2$O 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% 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 \(Q(H_2O) = 1.7 \times 10^{20}\) 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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