THE DISTRIBUTION, EXCITATION, AND FORMATION OF COMETARY MOLECULES: METHANOL, METHYL CYANIDE, AND ETHYLENE GLYCOL

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ABSTRACT

We present an interferometric and single-dish study of small organic species toward Comets C/1995 O1 (Hale-Bopp) and C/2002 T7 (LINEAR) using the BIMA interferometer at 3 mm and the ARO 12 m telescope at 2 mm. For Comet Hale-Bopp, both the single-dish and interferometer observations of CH₃OH indicate an excitation temperature of 105 ± 5 K and an average production rate ratio Ω(CH₃OH)/Ω(H₂O) ~ 1.3% at ~1 AU. In addition, the aperture synthesis observations of CH₃OH suggest a distribution well described by a spherical outflow and no evidence of significant extended emission. Single-dish observations of CH₃CN in Comet Hale-Bopp indicate an excitation temperature of 200 ± 10 K and a production rate ratio of Ω(CH₃CN)/Ω(H₂O) ~ 0.017% at ~1 AU. The nondetection of a previously claimed transition of cometary (CH₃OH)₂ toward Comet Hale-Bopp with the 12 m telescope indicates a compact distribution of emission, D < 9″ (<8500 km). For the single-dish observations of Comet T7 LINEAR, we find an excitation temperature of CH₃OH of 35 ± 5 K and a CH₃OH production rate ratio of Ω(CH₃OH)/Ω(H₂O) ~ 1.5% at ~0.3 AU. Our data support current chemical models that CH₃OH, CH₃CN, and (CH₃OH)₂ are parent nuclear species distributed into the coma via direct sublimation of cometary ices from the nucleus with no evidence of significant production in the outer coma.

Subject headings: astrobiology — comets: individual (Hale Bopp [C/1995 O1], LINEAR [C/2002 T7]) — molecular processes — radio lines: solar system — techniques: interferometric

1. INTRODUCTION

Over the last several years, complementary observations of comets with both single-dish telescopes and interferometric arrays have shed new light on the abundance, production rate, distribution, and formation of molecules in cometary comae. Recently, Milam et al. (2006) employed this method to investigate the origins of cometary formaldehyde (H₂CO) by comparing observations with both the Arizona Radio Observatory (ARO) 12 m single-dish telescope and the Berkeley-Illinois-Maryland Association (BIMA) array. From this investigation toward Comet C/1995 O1 (Hale-Bopp), the authors clearly showed that the distribution and abundance of H₂CO must be coming from a source other than the comet nucleus. The extended source of H₂CO may be due to enhanced production of this molecule (~4 times larger) from grains consisting of silicates and organic material (Milam et al. 2006), or possibly from the photodissociation of a larger parent species such as methanol (CH₃OH; Hudson et al. 2005). These complementary observations, however, are very difficult to obtain, as most of the molecular observations toward comets are performed using solely single-dish telescopes or interferometric arrays, depending on the telescope available at the time as the comet approaches the inner solar system and perigee.

Multiple facility collaborations for cometary observations are necessary if we are to further understand the formation, excitation, and distribution of organic cometary material. Recent cometary models of the abundance of organic material suggest Oort Cloud comets may have had their origin in the giant planet region, where they were thermally and chemically processed, before being ejected into the Oort Cloud (Weissman 1999). Furthermore, observations comparing long- and short-period comets suggest distinct classes: organic “rich,” “normal,” and “depleted” (Bowell et al. 2008; Mumma et al. 2003). However, the current sample size is too limited to accurately characterize each class of comets. It should also be noted that many of the comets described as organic “rich” have undergone breakup or fragmentation events, thus exposing more internal, unprocessed material than an object just entering the inner solar system (Bowell et al. 2008). So, the question persists, how does the classification of organic “rich,” “normal,” or “depleted” hold with regard to comets that, for example, are dust-rich versus dust-poor, have undergone a recent breakup, or bear high abundances of hypervolatile species?

The organic species examined in this study, methanol (CH₃OH), methyl cyanide (CH₃CN), and ethylene glycol [(CH₂OH)₂], are believed to be parent species directly sublimated off the cometary
ices in the nucleus. Since the first reported single-dish detections of cometary CH$_3$OH toward Comet Brosens-Metcalf (1989 o) and Comet Austin (1989 c1) (Colom et al. 1990), CH$_3$OH remains the most abundant large (>5 atoms) organic (containing a C atom) molecule measured in cometary ices. In a recent review by Charnley & Rodgers (2008), CH$_3$OH has a measured abundance range relative to H$_2$O between 1% and 4%. However, aperture synthesis observations of cometary CH$_3$OH are very rare, and no high spatial resolution data of this molecule currently exist. Similarly, single-dish observations of CH$_3$CN and (CH$_2$OH)$_2$ also suggest a purely nuclear origin (Biver et al. 2002; Crovisier et al. 2004). CH$_3$CN and HC$_3$N may be parent species that would increase the abundance of the CN radical, as well as C$_2$ in the coma. Yet, current observations do not preclude the possibility of CH$_3$CN having its own parent species (Bockelée-Morvan et al. 1987). In addition, the high abundance of (CH$_2$OH)$_2$, observed in Comet Hale-Bopp at high spatial resolution also strongly suggests a nuclear origin. To date, complementary observations of the same transitions of either CH$_3$CN or (CH$_2$OH)$_2$ with another facility were not available to follow up on the claimed distribution of these species in the coma and their possible formation pathways.

In this paper, we report on complementary observations of cometary CH$_3$OH, CH$_3$CN, and (CH$_2$OH)$_2$ taken with the BIMA array near Hat Creek, California, and the ARO 12 m telescope on Kitt Peak, Arizona, toward Comets C/1995 O1 (Hale-Bopp) and C/2002 T7 (LINEAR). From these observations, we continued to investigate the abundance, production rate, distribution, and formation of molecules in comets by directly comparing the measurements of these organic species with different telescopes. Our data support the hypothesis that CH$_3$OH, CH$_3$CN, and (CH$_2$OH)$_2$ are primarily parent species, generated by direct sublimation of cometary ices contained in the nucleus.

2. OBSERVATIONS

2.1. BIMA Array

Our observations of Comet Hale-Bopp with the BIMA array constitute one of the earliest detections of cometary CH$_3$OH with an interferometer. These measurements were taken using the “soft” C configuration of the BIMA array from 1997 March 24 to April 3. Data were acquired in the interferometric (cross-correlation) mode with nine antennas. The minimum baseline for these observations was ~15 m, and the maximum baseline was ~139 m. The average resulting full width at half-power synthesized beam size was ~8$''$ x 10$''$ for the observations. The quasar 0102+584 was used to calibrate the antenna-based gains, and the absolute amplitude calibration of this source was based on planetary observations and is accurate to within ~20%. The spectral windows containing the transitions had a bandwidth of 25 MHz and were divided into 256 channels for a spectral resolution of 0.1 MHz per channel. However, to increase the signal-to-noise ratio (S/N) in each window, the data were averaged over two channels, giving an effective spectral resolution of 0.2 MHz per channel. All data were first corrected to JPL ephemeris reference orbit 139. The data were then combined and imaged using the MIRIAD software package (Sault et al. 1995). To include all the data from the comet with multiple tracks, the data were inverted in u-v space. The resulting synthesized beam size was determined from the combined data set. The u-v data from multiple tracks were combined to make images. Table 1 summarizes the observational parameters of the BIMA array observations.

### Table 1

<table>
<thead>
<tr>
<th>Frequency (GHz)</th>
<th>Observation Date (UT)</th>
<th>$\Delta$ (AU)</th>
<th>$e$ (AU)</th>
<th>Beam (Jy beam$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>96.741</td>
<td>1997 Mar 27</td>
<td>1.323</td>
<td>0.919</td>
<td>10.8 x 8.2</td>
</tr>
<tr>
<td>107.014</td>
<td>1997 Mar 31</td>
<td>1.344</td>
<td>0.914</td>
<td>9.8 x 7.8</td>
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<td>1997 Mar 26</td>
<td>1.320</td>
<td>0.921</td>
<td>19.3 x 6.8</td>
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<tr>
<td></td>
<td>1997 Apr 2</td>
<td>1.359</td>
<td>0.914</td>
<td>11.7 x 6.6</td>
</tr>
<tr>
<td></td>
<td>1997 Apr 3</td>
<td>1.367</td>
<td>0.915</td>
<td>16.0 x 6.4</td>
</tr>
</tbody>
</table>

2.2. 12 m Single Dish

Observations at 2 mm of CH$_3$OH, CH$_3$CN, and (CH$_2$OH)$_2$ toward Comet Hale-Bopp were taken during three observing runs on 1997 March 10, 11, and 20 using the ARO (at the time, NRAO)$^{14}$ 12 m telescope. Observations of CH$_3$OH toward Comet LINEAR were conducted on 2004 May 20, also using the ARO 12 m telescope. Dual-channel SIS mixers were used for the 2 mm observations, operated in single-sideband mode with ~20 dB image rejection. The back ends employed for the presented observations were individual filter banks with 500 kHz resolution and the millimeter autocorrelator (MAC) with a resolution of 781 kHz. The spectral temperature scale was determined by the chopper-wheel method, corrected for forward spillover losses, and given in terms of $T_B$ (K). The radiation temperature, $T_R$, is then derived from the corrected beam efficiency, $\eta_B$, where $T_B = T_R/\eta_B$. A two-body ephemeris program was used to determine the comet’s position using the orbital elements provided by D. Yeomans (1996, private communication) of JPL for Comet Hale-Bopp, and JPL ephemeris reference orbit 69 was used for the Comet LINEAR observations. Focus and positional accuracy were checked periodically on nearby planets or maser sources. Data were taken in the position-switched mode with the off position 30$''$ west in azimuth. Observing frequencies, dates, comet geocentric and heliocentric distances, beam size, the diameter of the projected beam size on the comet, and the corrected main beam efficiency ($\eta_B$) at the times of observation are listed in Table 2.

3. RESULTS

3.1. BIMA Array

Figure 1 shows the images and spectra of CH$_3$OH taken toward Comet Hale-Bopp with the BIMA array. Figure 1a shows

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$^{14}$ The National Radio Astronomy Observatory is a facility of the National Science Foundation operated under cooperative agreement by Associated Universities, Inc.

$^{15}$ Available at http://www.splatalogue.net.
### TABLE 2

**Observational Parameters: ARO 12 m**

<table>
<thead>
<tr>
<th>Frequency (GHz)</th>
<th>Observation Date (UT)</th>
<th>Δ (AU)</th>
<th>r (AU)</th>
<th>Beam (arcsec)</th>
<th>D (km)</th>
<th>ηc</th>
<th>Molecule</th>
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<td>145.766</td>
<td>1997 Mar 20.94</td>
<td>1.318</td>
<td>0.940</td>
<td>43</td>
<td>41105</td>
<td>0.76</td>
<td>CH$_3$OH</td>
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<tr>
<td>147.105</td>
<td>1997 Mar 20.66</td>
<td>1.318</td>
<td>0.940</td>
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<td>41105</td>
<td>0.76</td>
<td>CH$_3$CN</td>
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<tr>
<td>148.112</td>
<td>1997 Mar 11.89</td>
<td>1.368</td>
<td>0.989</td>
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<td>41672</td>
<td>0.76</td>
<td>CH$_3$OH</td>
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<tr>
<td>150.142</td>
<td>1997 Mar 10.71</td>
<td>1.377</td>
<td>0.996</td>
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<td>151.860</td>
<td>1997 Mar 20.92</td>
<td>1.318</td>
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<td>CH$_3$OH</td>
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<td>157.049</td>
<td>1997 Mar 21.54</td>
<td>1.316</td>
<td>0.936</td>
<td>40</td>
<td>38179</td>
<td>0.72</td>
<td>CH$_3$OH</td>
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</table>

**Comet LINEAR**

<table>
<thead>
<tr>
<th>Frequency (GHz)</th>
<th>Observation Date (UT)</th>
<th>Δ (AU)</th>
<th>r (AU)</th>
<th>Beam (arcsec)</th>
<th>D (km)</th>
<th>ηc</th>
<th>Molecule</th>
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<tr>
<td>157.261</td>
<td>2004 May 21.80</td>
<td>0.284</td>
<td>0.865</td>
<td>40</td>
<td>8239</td>
<td>0.72</td>
<td>CH$_3$OH</td>
</tr>
</tbody>
</table>

* Average of observing frequencies between the K = 7 and K = 0 lines of CH$_3$CN.

*b* Average of observing frequencies of CH$_3$OH lines detected in the same spectral band.

Figure 1c shows the image of the $J(K_a, K_c) = 3(1, 3) - 4(0, 4)$ A transition of CH$_3$OH averaged over 3 days, 1997 March 26 and April 2 - 3. Figure 1d shows the spectrum of this CH$_3$OH transition near 107.0 GHz (Table 3). Note that the two CH$_3$OH emission contours shown in Figures 1a and 1c are centered on the predicted location of the comet nucleus with no apparent offset. The images are similar to each other and to the average of the March HCN BIMA array contours given by Veal et al. (2000) and the CO BIMA array contours given by Milam et al. (2006). In addition, there is no pronounced evidence for the jets or significant extended enhancement of CH$_3$OH beyond the 3 σ detection level (§ 4.2). Furthermore, from Figures 1b and 1d, there is no apparent second velocity component of CH$_3$OH, nor is the emission offset from the cometary rest velocity of 0 km s$^{-1}$.

### TABLE 3

**Molecular Line Parameters**

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Transition</th>
<th>Frequency$^a$ (GHz)</th>
<th>$\langle v_{LS} \rangle^2$ (D$^2$)</th>
<th>$A_{i,j}$ (s$^{-1}$)</th>
<th>$E_v$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_3$OH</td>
<td>$J(K_a, K_c) = 2(-1, -1) - 1(-1, 1)$ E</td>
<td>96,739.363(3)</td>
<td>1.2</td>
<td>2.55 x 10$^{-6}$</td>
<td>12.6</td>
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<tr>
<td>CH$_3$CN</td>
<td>$J(K_a) = 8(6) - 7(6)$</td>
<td>147,072.6082(2)</td>
<td>53.2</td>
<td>0.58 x 10$^{-4}$</td>
<td>289.0</td>
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<td>CH$_3$OH</td>
<td>$J(K_a, K_c) = 8(5) - 7(5)$</td>
<td>147,103.741(1)</td>
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<td>1.62 x 10$^{-4}$</td>
<td>210.5</td>
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<tr>
<td>CH$_3$OH</td>
<td>$J(K_a, K_c) = 8(4) - 7(4)$</td>
<td>147,129.232(1)</td>
<td>91.3</td>
<td>1.99 x 10$^{-4}$</td>
<td>146.2</td>
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<td>CH$_3$OH</td>
<td>$J(K_a, K_c) = 8(3) - 7(3)$</td>
<td>147,149.068(1)</td>
<td>104.6</td>
<td>1.14 x 10$^{-4}$</td>
<td>96.1</td>
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<tr>
<td>CH$_3$OH</td>
<td>$J(K_a, K_c) = 8(2) - 7(2)$</td>
<td>147,163.243(1)</td>
<td>114.1</td>
<td>2.49 x 10$^{-4}$</td>
<td>60.4</td>
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<tr>
<td>CH$_3$OH</td>
<td>$J(K_a, K_c) = 8(1) - 7(1)$</td>
<td>147,171.750(1)</td>
<td>119.8</td>
<td>2.61 x 10$^{-4}$</td>
<td>38.9</td>
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<tr>
<td>CH$_3$OH</td>
<td>$J(K_a, K_c) = 8(0) - 7(0)$</td>
<td>147,174.587(1)</td>
<td>121.7</td>
<td>2.66 x 10$^{-4}$</td>
<td>31.8</td>
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</table>

* Uncertainties in parentheses refer to the least significant digit and are 2 σ values (type A coverage; Taylor & Kuyatt 1994).

$^b$ Molecular line parameters of CH$_3$OH and CH$_3$CN taken from SLAIM; $Q_e = 1.27^{+1.0}_{-0.9}$ for CH$_3$OH and $Q_e = 3.97^{+2.0}_{-1.0}$ for CH$_3$CN.

$^c$ Molecular line parameters of (CH$_3$OH)$_2$ taken from CDMS (Müller et al. 2005). The energy levels are noted as $J(K_a, K_c, v)$, where $v$ is the quantum number associated with OH tunneling (Christen & Müller 2003).
3.2. 12 m Single Dish

Figure 2 shows the spectra of the five $\lambda \approx 2$ mm transitions of CH$_3$OH detected toward Comet Hale-Bopp with the 12 m telescope (Table 3). The UT date and spectral line quantum numbers of each observed transition are located at the top of each panel. As in the BIMA spectra, the spectral line labels correspond to the rest frequency located at the top left of the spectral window for a velocity of 0 km s$^{-1}$. The CH$_3$OH detections reported by the 12 m data are all E-type transitions. Similarly, Figure 3 shows the spectrum of a cluster of E-type transitions of CH$_3$OH centered around 157.3 GHz observed toward Comet LINEAR with the ARO 12 m telescope.

Finally, Figure 4 shows the spectrum taken at the frequency of the $J = 8-7$ ($K = 0-7$) transitions of the symmetric top species methyl cyanide (CH$_3$CN) toward Comet Hale-Bopp using the 12 m telescope. The $K = 0-6$ components are clearly present in these data. CH$_3$CN and other symmetric tops have properties that make them ideal probes of physical conditions of astronomical environments (see, e.g., Araya et al. 2005; Remijan et al. 2004; Hofner et al. 1996). As with CH$_3$OH, there are no apparent additional velocity components of CH$_3$CN or offset from the cometary rest velocity of 0 km s$^{-1}$.

Table 4 lists the molecular species that were searched for toward Comets Hale-Bopp and LINEAR at or near the cometocentric velocity (0 km s$^{-1}$). Least-squares Gaussian fits were made for each spectral line in order to obtain the peak intensities and line widths for the detected transitions. For those transitions not detected, the $1/\sigma$ rms noise level is given. The spectroscopic parameters used in determining the column densities and production rates are found in Table 3, and the formalism for calculating column densities and production rates is described in § 4.1.

4. ANALYSIS AND DISCUSSION

4.1. Excitation, Abundances, and Production Rates

Determining the best temperature, column density, and production rates of cometary molecules is important because these factors are essential to understanding the formation of cometary species. This includes the role of grains in molecule formation, the relative impact of warm versus cold gas-phase chemistry, or the importance of photodissociation in the production of daughter
species in the coma. In order to determine the temperatures and column densities of the region of the coma that contains the CH$_3$OH and CH$_3$CN emission, we assume that each region has uniform physical conditions, that the populations of the energy levels can be characterized by a Boltzmann distribution, and finally, that the emission is optically thin. The rotational temperature diagram method was not employed for this analysis because even small errors in the intensities and widths of inherently weak spectral lines can cause large errors in determining the temperature and total column density (see, e.g., Snyder et al. 2005). The complete formalism for these calculations using the BIMA array data can be found in Remijan et al. (2006), and for the 12 m data it can be found in Milam et al. (2006).

Figure 1 shows the results of the model fit (blue line) applied to the CH$_3$OH BIMA array data toward Comet Hale-Bopp. The array data are well fit by an excitation temperature of $T_{\text{ex}} = 105 \pm 5$ K and a total beam-averaged column density of $N_T = (9 \pm 1) \times 10^{14}$ cm$^{-2}$, assuming that the CH$_3$OH emission is extended beyond the 10.33$'' \times 8.46''$ average synthesized beam of the BIMA array (i.e., the beam filling factor, $f = 1$). Similarly, Figure 2 shows the results of the model fit applied to the CH$_3$OH ARO 12 m data with the same excitation temperature and a slightly lower column density of $N_T = (2.4 \pm 0.3) \times 10^{14}$ cm$^{-2}$. The average total column density from these two facilities is $N_T = (5.7 \pm 0.7) \times 10^{14}$ cm$^{-2}$. As the figure shows, the modeling reproduces the observations. Assuming that CH$_3$OH is a parent species, production rates were determined from a Monte Carlo model for a nuclear source (see Combi & Smyth 1988). This model traces the trajectories of molecules within the telescope beam ejected from the comet surface. The observed column density is then matched for an output molecular production rate, $Q$ (s$^{-1}$). Input parameters include the lifetime of the molecule...
from Huebner et al. (1992) scaled by \( k_B T \), the outflow velocity, the telescope beam size, and the observed column density. Assuming a nuclear origin for CH\(_3\)OH and using this Monte Carlo model, we find an average CH\(_3\)OH production rate from both instruments of \( Q(\text{CH}_3\text{OH}) \approx 1.3 \times 10^{29} \text{ s}^{-1} \) or \( Q(\text{CH}_3\text{OH})/Q(\text{H}_2\text{O}) \approx 1.3\% \) at \( \sim 1 \text{ AU} \). This production rate ratio assumes \( Q(\text{H}_2\text{O}) = 10^{31} \text{ s}^{-1} \) (Crovisier et al. 2004).

In Figure 2, there is a slight discrepancy between the observed intensities and model predictions for the CH\(_3\)OH lines at 151.86 GHz. The model predicts a higher line intensity than observed and underestimates the line intensity at 148.11 and 145.76 GHz. However, given the S/N of all the passbands where these lines are observed, the model does a very good job of predicting the expected line intensity of each CH\(_3\)OH transition observed with the 12 m telescope. The same can be said for the array data. The only discrepancy is the 96.74 GHz transition \( J(K_a, K_v) = 2(0,2)–1(0,1) \) CH\(_3\)OH transition (Fig. 1); the intensity is somewhat underestimated by our model fit.

Figure 4 shows the best model fit to the \( J(K_a) = 8(8)–7(7) \) (\( K = 0–6 \)) transitions of methyl cyanide (CH\(_3\)CN) toward Comet Hale-Bopp. Once again, the blue line shows the model predictions for the CH\(_3\)CN data which are best fit by an excitation temperature of \( T_{ex} = 200 \pm 10 \text{ K} \) and a total beam-averaged column density of \( N_T = (2.6 \pm 0.3) \times 10^{12} \text{ cm}^{-2} \). In this case, the predicted \( K = 7 \) line intensity is below the 1 \( \sigma \) detection limit, which indicates that the emission feature near the \( K = 7 \) rest frequency may not be real. Assuming a nuclear origin for CH\(_3\)CN and using a Monte Carlo model, we find a production rate of \( Q(\text{CH}_3\text{CN}) \sim 1.7 \times 10^{27} \text{ s}^{-1} \) or \( Q(\text{CH}_3\text{CN})/Q(\text{H}_2\text{O}) \approx 0.017\% \) at \( \sim 1 \text{ AU} \). This production rate is similar to what Biver et al. (1997) found, \( \sim 10^{27} \text{ s}^{-1} \) at 1 AU, in their study.

These 12 m data overlap in frequency with the (CH\(_3\)OH)\(_2\) IRAM 30 m study of Crovisier et al. (2004). In the IRAM data set, the claimed detection of the \( J(K_a, K_v) = 15(7, 9, 0)–14(7, 8, 1) \) and \( 15(7, 8, 0)–14(7, 7, 1) \) transitions at 147.13 GHz are nearly coincident in frequency and show up as one feature given the spectral resolution. Moreover, the (CH\(_3\)OH)\(_2\) transitions have an overall line intensity equal to that of the \( J(K_a) = 8(4)–7(4) \) transition of CH\(_3\)CN detected with the IRAM 30 m telescope. From the ARO 12 m data, we identify the same spectral features of CH\(_3\)CN but do not detect any emission from the two transitions of (CH\(_3\)OH)\(_2\) below the 1 \( \sigma \) limit. From the CH\(_3\)CN, CH\(_3\)OH, and (CH\(_3\)OH)\(_2\) 12 m data, it is clear we are probing different physical environments in the coma of Comet Hale-Bopp. A discussion of the distribution of these molecular species is in \( \S \) 4.2.

Figure 3 shows the best model fit (blue line) to the cluster of \( E \)-type transitions of CH\(_3\)OH centered around 157.26 GHz toward Comet LINEAR with the ARO 12 m telescope. There have been very few molecular line observations toward Comet LINEAR. The most complete study of molecular species toward this object was by Remijan et al. (2006) using the BIMA array. These authors detected the \( J(K_a, K_v) = 3(1, 3)–4(0, 4) \) transition of CH\(_3\)OH with a synthesized beam size of 22.3\" \( \times \) 16.9\". Using the proposed excitation temperature of 115 K (DiSanti et al. 2004; Magee-Sauer et al. 1999; Küppers et al. 2004), Remijan et al. determined a total beam-averaged column density for CH\(_3\)OH of \( N_T = (1.4 \pm 0.3) \times 10^{14} \text{ cm}^{-2} \). However, as shown in Figure 3, the 12 m CH\(_3\)OH data are best fit by an excitation temperature of...
Fig. 5.—CH$_3$OH transitions from Comet LINEAR and the model fit to the data (blue line) from the BIMA array data. Top: Hanning-smoothed data. Bottom: Raw data. See text.

$T_{ex} = 35 \pm 5$ K and a total beam-averaged column density of $N_T = (2.2 \pm 0.3) \times 10^{17}$ cm$^{-2}$ (blue line), implying a production rate of $Q$(CH$_3$OH) $\sim 2.0 \times 10^{27}$ s$^{-1}$ or $Q$(CH$_3$OH)/$Q$(H$_2$O) $\sim$ 1.5% at 0.3 AU. This production rate ratio assumes $Q$(H$_2$O) = $1.3 \times 10^{29}$ s$^{-1}$ (Lecacheux et al. 2004). To reconcile the differing column density determined by Remijan et al. (2006), we used the best model fit parameters of temperature and column density from the 12 m data to predict the line intensity of the $J(K_a, K_c) = 3(1,3)\rightarrow 4(0,4)$ $A^+$ transition detected by the BIMA array. Figure 5 shows the result of this analysis (the top panel shows the Hanning-smoothed data, and the bottom panel shows the raw data as in Fig. 1 of Remijan et al. [2006]). The fit is excellent. From using the ARO data it is quite clear that the assumption of an excitation temperature of $T_{ex} = 115$ K for CH$_3$OH was incorrect, and the determined column density of CH$_3$OH toward Comet LINEAR was therefore overestimated by almost an order of magnitude.

4.2. Distribution of Molecular Species

We present two complementary sets of data from Comet Hale-Bopp that give great insights into the distribution of CH$_3$OH, CH$_3$CN, and (CH$_3$OH)$_2$. First, it is quite clear from the data presented in Figures 1 and 2 that despite the drastic change in the telescope beam sizes between the array and the 12 m telescope, we are still sampling a region of the coma that is thermalized to $\sim$105 K. The ratio of areas subtended by the 12 m beam compared to the BIMA array synthesized beam is $\sim$21:1, which corresponds to a change in the physical sampled size scale from $D \sim 40,000$ to 8500 km. A direct comparison of the column densities from the 12 m telescope and BIMA array suggest an enhancement of the CH$_3$OH abundance at smaller coma radii. Furthermore, column (5) in Table 3 lists the Einstein $A$ coefficients for each transition of CH$_3$OH, CH$_3$CN, and (CH$_3$OH)$_2$. Assuming a collision cross section of $\sim 10^{-15}$ cm$^2$ and a temperature of 105 K, the calculated critical densities of the detected CH$_3$OH transitions are in the range $(0.7\sim 3.2) \times 10^5$ cm$^{-3}$. Our observations encompass a region with a H$_2$O density of $\sim 10^{5.5\sim 7.5}$ cm$^{-3}$ (Lovell et al. 2004). Therefore, there is sufficient collisional excitation to populate the CH$_3$OH levels, and our observations sample molecular abundances and not excitation effects.

Figure 6a once again shows the distribution of the $J(K_a, K_c) = 3(1,3)\rightarrow 4(0,4)$ $A^+$ transition of CH$_3$OH around Comet Hale-Bopp. Figure 6b is a model fit to the data shown in Figure 6a. The model was generated assuming a spherical Haser model of parent species sublimating off the comet’s nucleus. From the data in Figure 6a, the scale length of the distribution of CH$_3$OH around the nucleus is measured to be $r \sim 10''$. Using this scale length and the MIRIAD task IMGEN, a Haser model distribution of CH$_3$OH was generated, which was then convolved with the synthesized beam of the BIMA array (Fig. 6, bottom left of each panel). The residuals obtained by subtracting the model from the data are shown in Figure 6c. While it appears that there may be a more extended distribution of CH$_3$OH detected by the BIMA array based on the residual data, it is important to note that the
contour levels shown in Figures 6a and 6b are 3, 4, 5, and 6 \( \sigma \) (\( \sigma = 0.05 \text{ Jy beam}^{-1} \)), whereas the data shown in Figure 6c are 1 and 1.5 \( \sigma \). Although there is some indirect evidence for an extended distribution of CH\(_2\)OH with \( D = 40,000 \text{ km} \) from the 12 m detections of CH\(_2\)OH, the data presented in Figure 6c indicate that any extended emission is completely resolved out by the array. The array would be sensitive to extended emission of CH\(_2\)OH in the outer coma only if the distribution were “clumpy,” as is seen in H\(_2\)CO (Milam et al. 2006).

It appears that CH\(_3\)CN is tracing higher temperature and higher density gas than CH\(_2\)OH. Because CH\(_3\)CN has a larger dipole moment than CH\(_2\)OH, its measured excitation should be lower, given identical conditions. However, if the overall distribution of CH\(_3\)CN is closer to the nucleus than CH\(_2\)OH, we would expect to measure a higher excitation temperature (it is well known that the temperature of the coma increases with decreasing coma radii; Biver et al. 1999). This distribution would also imply that CH\(_3\)CN is a parent species (\( \S \) 4.3). Given the difference in beam sizes between the 12 and 30 m telescopes, we can get an estimate of the size of the emitting region based on the relative beam sizes using the beam filling factor in the expression for column density. Comparing the relative line intensities between the \( K = 3 \) and 4 transitions of CH\(_3\)CN from the IRAM 30 m data and what is measured from the 12 m telescope, the 30 m emission features from CH\(_3\)CN are \( \sim 5-10 \text{ times stronger than what is observed from the 12 m telescope.} \) This difference implies either (1) an enhancement of the CH\(_3\)CN column density at smaller coma radii or (2) that the excitation of the transitions we observed of CH\(_3\)CN takes place at a slightly smaller radius, where the density is higher, and the measurements taken with the 12 m telescope are suffering from some beam dilution. Assuming the H\(_2\)O density profile of Lovell et al. (2004), the maximum coma radius that lies below the CH\(_3\)CN critical density range of \( (1.2-5.3) \times 10^{6} \text{ cm}^{-3} \) is \( \sim 10,000 \text{ km}. \) This explains why the 30 m CH\(_3\)CN line strengths are higher than the 12 m. Finally, from the nondetection of (CH\(_3\)OH)\(_2\) in the 12 m observations, it is also apparent that the distribution of (CH\(_3\)OH)\(_2\) must also be compact in the coma. Assuming that the detected transition line strength of \( \sim 0.09 \text{ K} \) in the 30 m spectrum is from (CH\(_3\)OH)\(_2\) and a 1 \( \sigma \) line intensity of \( \sim 0.01 \text{ K} \) in the 12 m passband, the emission from (CH\(_3\)OH)\(_2\) must be on the order of \( D < 9'' \), corresponding to a physical size of \( D < 8500 \text{ km}. \) High-sensitivity, high-resolution interferometer observations are necessary to confirm this distribution.

4.3. Formation of Cometary Methanol and Other Molecular Species

From the high-resolution methanol observations of the BIMA array, it is clear that CH\(_2\)OH is either sublimating directly off the cometary ices contained in the nucleus or is formed very deep in the cometary coma. If CH\(_3\)OH originates in the ices, this molecule may be a remnant of the formation of the presolar nebula and hence the interstellar medium. Currently, there are two accepted formation pathways to the interstellar production of CH\(_3\)OH, including the radiative association of CH\(_3\)^+ + H\(_2\)O \( \rightarrow \) CH\(_3\)O\(_2\)^+, followed by recombination with an electron to produce CH\(_3\)OH and H (Herbst 1985). Grain surface reactions that involve the repeated hydrogenation of CO \( \rightarrow \) H + CO \( \rightarrow \) HCO + H \( \rightarrow \) HCHO \( \rightarrow \) HCHO are thought to eventually lead to CH\(_3\)OH (Hiraoka et al. 1994). Our observations show that there is no significant enhancement in the production of CH\(_3\)OH in the outer coma as the comet enters the inner solar system.

The same argument can be applied to CH\(_3\)CN. The accepted route to the formation of CH\(_3\)CN in interstellar environments is CH\(_3\)^+ + HCN. A collision complex is formed that equilibrates to CH\(_3\)CNH\(^+\) + \( \nu \) (Herbst 1985), then CH\(_3\)CNH\(^+\) combines with an electron to form CH\(_3\)CN + H. Our observations of CH\(_3\)CN show that it is currently close to the cometary nucleus, indicating direct sublimation off cometary ices. However, the excitation of the transitions we observed of CH\(_3\)CN takes place at a smaller radius where the density is higher, and this molecule may be present as well at larger radii. However, the true spatial scale and scale length of CH\(_3\)CN need to be verified by interferometric observations.

Finally, the nondetection of (CH\(_3\)OH)\(_2\) with the ARO 12 m telescope gives insight into the formation of (CH\(_3\)OH)\(_2\), as well as the possibility of detecting CH\(_2\)OHCHO. If the transition detected by the 30 m telescope is indeed from cometary (CH\(_3\)OH)\(_2\), in \( \S \) 4.2, we found that the predicted distribution of (CH\(_3\)OH)\(_2\) toward Comet Hale-Bopp was calculated to be \( D < 9'' (\sim 8500 \text{ km} \) again suggesting direct sublimation off cometary ices or enhanced production in the inner coma. Presumably, as with the formation of CH\(_2\)OH and CH\(_3\)CN in interstellar environments, (CH\(_3\)OH)\(_2\) would be formed in the interstellar medium and then seeded into cometary ices. Currently, there is no accepted gas-phase interstellar formation mechanism that can lead to the production of (CH\(_3\)OH)\(_2\). However, there are several formation pathways using surface chemistry which may occur on icy grain mantles. For example, to form (CH\(_3\)OH)\(_2\) and CH\(_2\)OHCHO, formaldehyde (H\(_2\)CO) produces CH\(_2\)OHCHO in an aqueous Formose reaction, which can then be hydrogenated to form (CH\(_3\)OH)\(_2\) (e.g., see Walker 1975). Charnley (2001) predicts that (CH\(_3\)OH)\(_2\) and CH\(_2\)OHCHO could be formed by direct hydrogenation reactions, starting from ketene (CH\(_2\)CO) on grain surfaces. Finally, Hudson & Moore (2000) show that proton-irradiated CH\(_2\)OH on icy interstellar grain mantles can lead to the formation of (CH\(_3\)OH)\(_2\). Thus, there appear to be several ways to form and embed (CH\(_3\)OH)\(_2\) into cometary ices.

5. Conclusions

We present an interferometric and single-dish study of cometary molecules toward comets C/1995 O1 (Hale-Bopp) and C/2002 T7 (LINEAR) using the Berkeley-Illinois-Maryland Association (BIMA) interferometer at 3 mm and the Arizona Radio Observatory (ARO) 12 m telescope at 2 mm. The overall conclusions from our analysis of these data are as follows:

1. The CH\(_2\)OH Hale-Bopp data are well fit by an excitation temperature of \( T_{\text{ex}} = 105 \pm 5 \text{ K} \) and a total beam-averaged column density of \( N_{T} = (5.7 \pm 0.7) \times 10^{14} \text{ cm}^{-2} \). Assuming a nuclear origin for CH\(_2\)OH and using a Monte Carlo model, we find an average CH\(_2\)OH production rate from both instruments of \( Q(\text{CH}_2\text{OH}) \sim 1.3 \times 10^{29} \text{ s}^{-1} \) or \( Q(\text{CH}_2\text{OH})/Q(\text{H}_2\text{O}) \sim 1.3\% \) at \( \sim 1 \text{ AU} \).

2. The CH\(_2\)OH ARO 12 m LINEAR data centered around 157.26 GHz are best fit by an excitation temperature of \( T_{\text{ex}} = 35 \pm 5 \text{ K} \) and a total beam-averaged column density of \( N_{T} = (2.2 \pm 0.3) \times 10^{13} \text{ cm}^{-2} \) and thus a production rate of \( Q(\text{CH}_2\text{OH}) \sim 2.0 \times 10^{27} \text{ s}^{-1} \) or \( Q(\text{CH}_2\text{OH})/Q(\text{H}_2\text{O}) = 1.5\% \) at \( 0.3 \text{ AU} \).

3. From the combination of the single-dish and aperture synthesis observations of CH\(_2\)OH, we find that the distribution of CH\(_2\)OH toward Comet Hale-Bopp is well described by a spherical outflow with an increase in column density closer to the cometary nucleus. The data presented in the array images show no evidence of significant enhanced production of CH\(_2\)OH in the extended coma or from jets, as any extended emission is completely resolved out by the array.
4. The CH$_3$CN 12 m Hale-Bopp data are best fit by an excitation temperature of $T_{ex} = 200 \pm 10$ K and a total beam-averaged column density of $N_T = (2.6 \pm 0.3) \times 10^{12}$ cm$^{-2}$. Assuming a nuclear origin for CH$_3$CN and using a Monte Carlo model, we find an average CH$_3$CN production rate of $Q$(CH$_3$CN) $\sim 1.7 \times 10^{27}$ s$^{-1}$ or $Q$(CH$_3$CN)/$Q$(H$_2$O) $\sim 0.017\%$ at $\sim$1 AU. A comparison between the single-dish observations from the ARO 12 m telescope and the IRAM 30 m telescope of CH$_3$CN suggest that the ARO observations are beam-diluted. The excitation of the observed transitions of CH$_3$CN takes place at a smaller radius where the density is higher and suggests a nuclear origin of CH$_3$CN.

5. The nondetection of a previously claimed transition of cometary (CH$_2$OH)$_2$ toward Comet Hale-Bopp with the ARO 12 m telescope indicates a compact distribution of emission on the order of $<9^\prime$ (<8500 km). This supports the hypothesis that the cometary production of (CH$_2$OH)$_2$ is via direct sublimation off cometary ices from the nucleus.

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