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# NEW MOLECULAR SPECIES IN COMET C/1995 O1 (HALE-BOPP) OBSERVED WITH THE CALTECH SUBMILLIMETER OBSERVATORY

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**Abstract.**
We present millimeter-wave observations of HNCO, $HC_3N$, SO, $NH_2CHO$, $H^{13}CN$, and $H_3O^+$ in comet C/1995 O1 (Hale-Bopp) obtained in February–April, 1997 with the Caltech Submillimeter Observatory (CSO). HNCO, first detected at the CSO in comet C/1996 B2 (Hyakutake), is securely confirmed in comet Hale-Bopp via observations of three rotational transitions. The derived abundance with respect to $H_2O$ is $(4 - 13) \times 10^{-4}$. $HC_3N$, SO, and $NH_2CHO$ are detected for the first time in a comet. The fractional abundance of $HC_3N$ based on observations of three rotational lines is $(1.9 \pm 0.2) \times 10^{-4}$. Four transitions of SO are detected and the derived fractional abundance, $(2 - 8) \times 10^{-3}$, is higher than the upper limits derived from UV observations of previous comets. Observations of $NH_2CHO$ imply a fractional abundance of $(1-8) \times 10^{-4}$. $H_3O^+$ is detected for the first time from the ground. The $H^{13}CN$ $(3-2)$ transition is also detected and the derived $HCN/H^{13}CN$ abundance ratio is $90 \pm 15$, consistent with the terrestrial $^{12}C/^{13}C$ ratio. In addition, a number of other molecular species are detected, including HNC, OCS, $HCO^+$, $CO^+$, and CN (the last two are first detections in a comet at radio wavelengths).

**Key words:** comets: composition; radio observations; spectroscopy

## 1. Introduction

The appearance of comet C/1995 O1 (Hale-Bopp) offered a rare opportunity to probe with unprecedented sensitivity the inner atmosphere of a comet and to investigate its chemical composition. With the recent improvements in the quality of telescopes and receivers operating at millimeter and submillimeter wavelengths, this wavelength range has been playing an increasingly important role in studies of the volatile composition of comets (e.g. Lis et al. 1997). In the present paper we

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summarize results of the observational campaign of comet Hale-Bopp organized at the CSO concerning new molecular species, ions, and isotopic ratios. Preliminary estimates of molecular abundances are presented. CSO observations of "classical" species are included in the long term monitoring of the gas production rates (Biver et al., 1998).

## 2. Observations

Observations of Comet C/1996 O1 (Hale-Bopp) presented here were carried out between Feb. 17 and Apr. 21, 1997 using the 10.4–m Leighton telescope of the CSO at the summit of Mauna Kea, Hawaii. CSO facility receivers, spectrometers, and calibration procedures are described in Lis et al. (1997). A list of the most interesting transitions detected at the CSO in comet Hale-Bopp is given in Table I along with the derived production rates for some of the new species. All fractional abundances with respect to $H_2O$ given in § 3 have been calculated using HCN production rates of Biver et al. (1998) and assuming an HCN fractional abundance of $3 \times 10^{-3}$ with respect to $H_2O$.

## 3. Results

### 3.1. Isocyanic Acid (HNCO) and Formamide ($NH_2CHO$)

Isocyanic acid, an important constituent of interstellar grains, was first detected in comet Hyakutake (Lis et al., 1997). A single rotational transition was detected implying an abundance with respect to $H_2O$ of $\sim 7 \times 10^{-4}$. In comet Hale-Bopp three rotational transitions of HNCO are detected (Table I). High-resolution spectra of the $(11_{0,11} - 10_{0,10})$ and $(12_{0,12} - 11_{0,11})$ lines are shown in Fig. 1 (left and middle panels, respectively). The HNCO abundance is $(4 - 13) \times 10^{-4}$ and appears to be decreasing monotonically over the period of two days. The HCN production rate increases by a factor of $\sim 1.7$ over the same period.

Two transitions of formamide are detected with the CSO and IRAM 30–m telescopes (Bockelée-Morvan et al., 1998). The derived fractional abundance, $(1 - 8) \times 10^{-4}$, depends strongly on the assumed photodissociation rate, $\beta$. The low value, corresponding to $\beta = 5 \times 10^{-5}$ s$^{-1}$, gives consistent production rates for the two transitions observed.

### 3.2. Cyanoacetylene ($HC_3N$)

A $3\sigma$ upper limit for the fractional abundance of cyanoacetylene in comet Hyakutake was $3.5 \times 10^{-4}$ (Lis et al., 1997). Three rotational

Table I. Selected CSO Observations of Comet Hale-Bopp

| Molecule | Transition | Frequency | UT Date | $\int T_R^* dv$ | $\sigma$ | $Q/10^{26}$ |
|---|---|---|---|---|---|---|
| HNCO | $11_{0,11} - 10_{0,10}$ | 241.774 | Feb 18.7 | 0.27 | 0.04 | 33 |
| | $12_{0,12} - 11_{0,11}$ | 263.749 | Feb 19.7 | 0.18 | 0.02 | 20 |
| | $16_{0,16} - 15_{0,15}$ | 351.633 | Feb 17.7 | 0.46 | 0.08 | 41 |
| $HC_3N$ | 24–23 | 218.325 | Feb 20.7 | 0.24 | 0.03 | 10 |
| | 28–27 | 254.700 | Feb 21.7 | 0.26 | 0.03 | 11 |
| | 29–28 | 263.792 | Feb 19.7 | 0.19 | 0.03 | 8 |
| SO | $5_5 - 4_4$ | 215.221 | Feb 20.7 | 0.11 | 0.02 | 136 |
| | $5_6 - 4_5$ | 251.826 | Feb 21.7 | 0.33 | 0.04 | 268 |
| | $7_6 - 6_5$ | 261.843 | Apr 21.3 | 0.56 | 0.07 | 345 |
| | $8_7 - 7_6$ | 304.078 | Feb 23.7 | 0.50 | 0.05 | 158 |
| OCS | 22–21 | 267.530 | Mar 26.7 | 0.50 | 0.06 | 250 |
| | 25–24 | 303.993 | Feb 23.7 | 0.15 | 0.03 | 470 |
| $H_3O^+$ | $3_2 - 2_2$ | 364.797 | Apr 6-10 | 0.38 | 0.07 | |
| $HCO^+$ | 3-2 | 267.558 | Mar 26.7 | 6.0 | 0.09 | |
| $CO^+$ | $2_{5/2} - 1_{3/2}$ | 236.063 | Feb 22.7 | 0.43 | 0.04 | |
| $NH_2CHO$ | $12_{5,7} - 11_{5,6}$ | 254.878 | Apr 5.8 | 0.070 | 0.009 | 100 |
| HNC | 4-3 | 362.630 | Feb 16.7 | 5.8 | 0.10 | |
| HCN | 4-3 | 354.505 | Feb 16.7 | 18.8 | 0.10 | |
| $H^{13}CN$ | 3-2 | 259.012 | Feb 19.7 | 0.27 | 0.02 | |
| HCN | 3-2 | 265.886 | Feb 19.7 | 23.0 | 0.08 | |
| CN | $2_{5/2} - 1_{3/2}$ | 226.875 | Feb 23.7 | 0.21 | 0.04 | |
| NaOH | 10 − 9 | 251.226 | Apr 20-21 | <0.07 | 0.024 | <0.3 |
| NaCl | 20 − 19 | 260.223 | Apr 16-17 | <0.17 | 0.057 | <0.8 |

Notes: Line frequencies are in GHz. Integrated line intensities and their uncertainties (in $\mathrm{K\,km\,s^{-1}}$) are corrected for main beam efficiencies of 72% and 65% (230 and 345 GHz receivers, respectively). Production rates (in $s^{-1}$) are computed assuming LTE at 80 K kinetic temperature (based on $CH_3OH$ observations) and a parent density distribution. The duration of the observations was typically $\sim 1-2^h$. NaOH and NaCl integrated intensities and production rates are $3\sigma$ upper limits.

transitions of $HC_3N$ detected in comet Hale-Bopp (Table I) provide the first identification of this species in a comet. The high-resolution spectrum of the $HC_3N$ (24–23) line is shown in Fig. 1 (right panel). The $HC_3N$ (28–27) spectrum taken with the wideband (500 MHz) spectrometer is shown in Fig. 2. The fractional abundance of $HC_3N$ relative to $H_2O$ based on our observations is $(1.9 \pm 0.2) \times 10^{-4}$, similar to that measured for $CH_3CN$ (Biver et al., 1998). The three transitions observed give consistent abundance values.

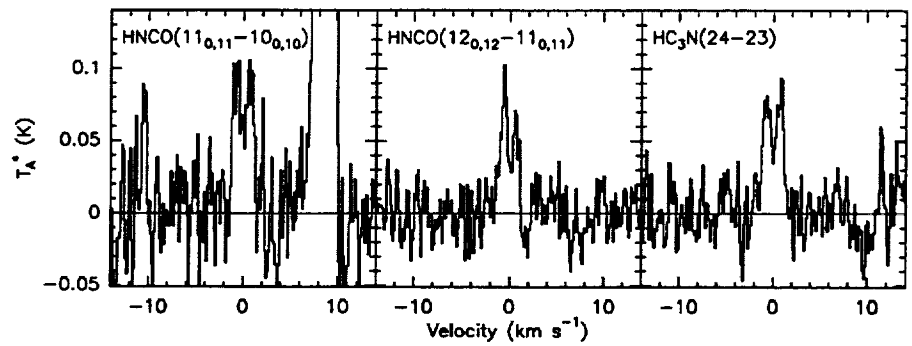


*Figure 1.* High-resolution spectra of HNCO ($11_{0,11} - 10_{0,10}$), HNCO ($12_{0,12} - 11_{0,11}$), and $HC_3N$ (24 − 23) in comet Hale-Bopp. The intensity scale is in antenna temperature units ($T_A^*$). The velocity scale is with respect to the comet rest velocity. The lines have characteristic double-peaked line shapes expected for optically thin isotropic outgassing. The strong line in the left panel is the 241.767 GHz transition of methanol.

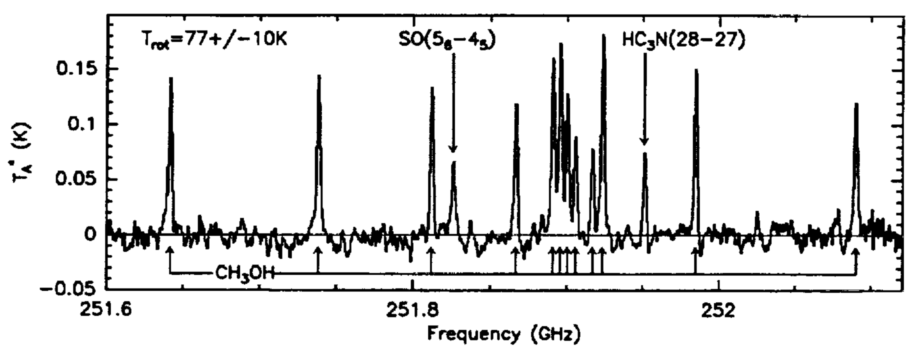


*Figure 2.* Wideband spectrum of the $HC_3N$ (28 − 27) line in comet Hale-Bopp (in the image sideband). A band of 12 methanol lines can also be seen, as well as the ($5_6 - 4_5$) line of SO. The rotational temperature based on the observed intensities of the 252 GHz methanol lines is $77 \pm 10$ K.

### 3.3. Sulfur Monoxide (SO)

Four rotational transitions of sulfur monoxide detected at the CSO in comet Hale-Bopp (Table I) provide the first identification of this species in a comet. Low- and high-resolution spectra of the ($5_6 - 4_5$) line are shown in Fig. 2 and 3 (left panel), respectively. Interferometric observations of the ($6_5 - 5_4$) line performed at IRAM show that SO does not have a parent molecule distribution and is produced by a short-lived species (Wink et al. 1998; see also Despois 1998), presumably $SO_2$ (Bockelée-Morvan et al., 1998). The fractional abundance of SO derived from our measurements is $(2 - 8) \times 10^{-3}$. The abundance is strongly model dependent, primarily due to the poorly constrained SO photodissociation rate, $\beta$. For a given value of $\beta$, the four measurements give consistent abundance values within the observational uncertainties. The production rates given in Table I correspond to $\beta = 4 \times 10^{-4}$ $s^{-1}$ and a parent density distribution.

Our derived SO abundance is much larger than the upper limits derived in comets C/IRAS-Araki-Alcock and P/Halley from UV observations (Kim and A'Hearn, 1991). As discussed by Kim et al. (1998), the SO abundances based on the UV upper limits were underestimated due to the wrong published SO line strengths in the UV.

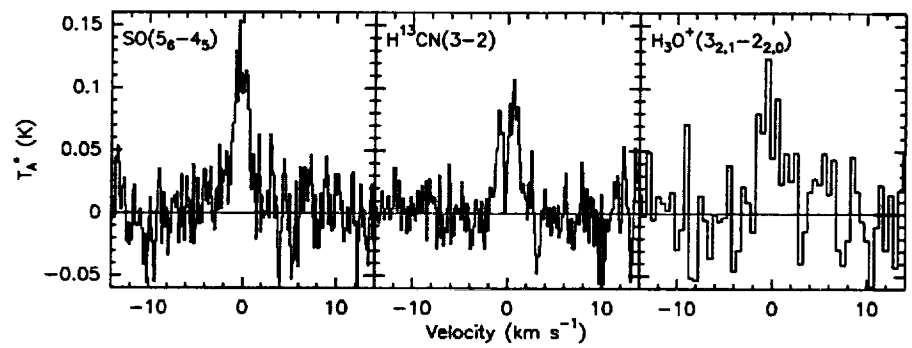


*Figure 3.* High-resolution spectra of SO ($5_6 - 4_5$), $H^{13}CN$ ($3-2$), and $H_3O^+$ ($3_2 - 2_2$) in comet Hale-Bopp.

### 3.4. $^{12}C/^{13}C$ Isotopic Ratio ($H^{13}CN$)

The $H^{13}CN$ ($4-3$) line was first detected in comet Hyakutake (Lis et al., 1997). The derived $HCN/H^{13}CN$ abundance ratio was $34 \pm 12$, significantly lower than the terrestrial $^{12}C/^{13}C$ ratio of 89. This low ratio may be in part due to contamination by an $SO_2$ line blended with the $H^{13}CN$ ($4-3$) line. To avoid possible contamination, we observed the $H^{13}CN$ ($3-2$) transition (Fig. 3, middle panel) for determination of the $HCN/H^{13}CN$ ratio in comet Hale-Bopp. The $HCN/H^{13}CN$ abundance ratio derived from our observations is $90 \pm 15$, consistent with the value measured by Jewitt et al. (1997), as well as the terrestrial $^{12}C/^{13}C$ abundance ratio.

### 3.5. Ions

Based on in situ measurements (Altwegg et al., 1993), $H_3O^+$ was the most abundant ion in the inner coma of comet P/Halley. Our observations of the $H_3O^+$ ($3_2 - 2_2$) line (Fig. 3, right panel) provide the first ground based detection of this species in a comet.

The $HCO^+$ emission (Fig. 4) is found to be strong and extended along the tail on scales larger than 300″ (290,000 km). The maximum

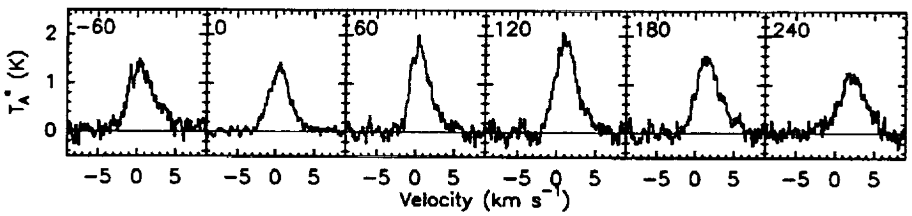


*Figure 4.* A strip map of $HCO^+$ emission along the tail. Offsets from the nucleus (in arcsec) are given in the upper-left corner of each panel.

intensity is not at the nucleus position, but ~100,000 km toward the tail direction. The observed variations in the line shape and line center velocity are caused by the acceleration of the ions by interactions with the solar wind magnetic field. These results are consistent with the observations of Lovell et al. (1998), Womack et al. (1998), and Bockelée-Morvan et al. (1998).

The $CO^+$ emission is detected for the first time at radio wavelengths (Fig. 5, left panel).

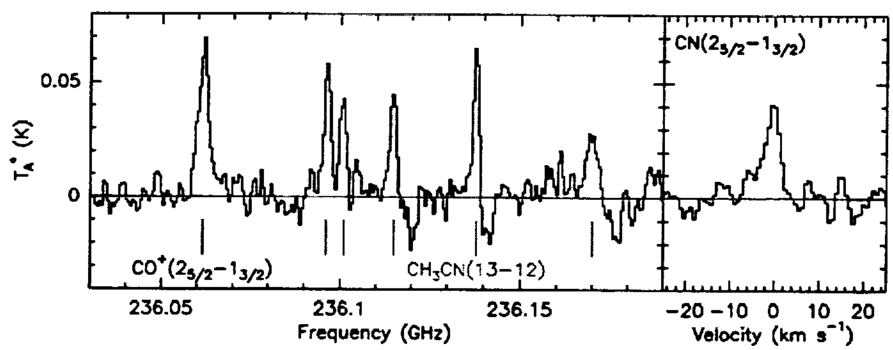


*Figure 5.* Spectra of $CO^+$ ($2_{5/2} - 1_{3/2}$) and CN ($2_{5/2} - 1_{3/2}$) in comet Hale-Bopp (left and right panels, respectively). Five lines of $CH_3CN$ from the image sideband can also be seen in the $CO^+$ spectrum.

### 3.6. Other Molecules

Numerous other molecular species are detected, including CN (Fig. 5, right panel; first detection at radio wavelengths). The HCN/HNC abundance ratio is found to be highly variable between Dec. 96 and Apr. 97 (this ratio varied between 4 and 17), suggesting that a significant fraction of HNC is produced in the coma (see Irvine et al. 1998). Another sulfur-bearing species, carbonyl sulfide (OCS), first detected in comet Hyakutake (Woodney et al., 1997), is securely confirmed via observations of two rotational transitions (Table I). The derived OCS abundance in comet Hale-Bopp is $\sim 6 \times 10^{-3}$, a factor of 6 higher than that in comet Hyakutake (Woodney et al., 1997).

In order to elucidate the origin of the release of sodium in comets, we searched for Na-bearing molecules (Table I). A comparison of our $3\sigma$ upper limit for the NaOH production rate derived on Apr. 20-21 (assuming a lifetime of $10^4$ s) with the Na production rate derived by Cremonese et al. (1997) for the sodium tail of comet Hale-Bopp suggests that NaOH is unlikely to be a parent of atomic sodium.

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