New Molecular Species in Comet C/1995 O1 (Hale-Bopp) Observed with the Caltech Submillimeter Observatory

D.C. Lis, D.M. Mehringer, D. Benford, M. Gardner and T.G. Phillips
Downs Laboratory of Physics 320–47, California Institute of Technology, Pasadena, CA 91125, USA

D. Bockelée-Morvan, N. Biver,* P. Colom and J. Crovisier
Observatoire de Paris, F–92195 Meudon Principal Cedex, France

D. Despois
Observatoire de Bordeaux, B.P. 89, F–33270, Floirac, France

H. Rauer
DLR, Berlin, Germany

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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 previous upper limits derived from UV observation. 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 ± 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

* Currently at the Institute for Astronomy, University of Hawaii.

composition of comets (e.g. Lis et al. 1997). In the present paper we summarize results of the observational campaign of comet Hale-Bopp organized at the CSO and give preliminary estimates of molecular abundances derived from our observations.

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 3×10^{-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 ~ 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, β. 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 3σ upper limit for the fractional abundance of cyanoacetylene in comet Hyakutake was 3.5×10^{-4} (Lis et al., 1997). Three rotational

Table I. Selected CSO Observations of Comet Hale-Bopp

Molecule	Transition	Frequency	UT Date	$\int T_R^* dv$	σ	$Q/10^{26}$
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 $\mathrm{K\,km\,s^{-1}}$) have been corrected for main beam efficiencies of 72% and 65% (230 and 345 GHz receivers, respectively). Production rates were 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 $\sim 1 - 2^{\mathrm{h}}$. Production rates of NaOH and NaCl are 3σ upper limits computed assuming a lifetime of 10^4 s.

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 (27–26) 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 $(1.9\pm0.2)\times10^{-4}$, similar to that measured for CH_3CN (Biver et al., 1998). The three transitions observed give consistent abundance values.

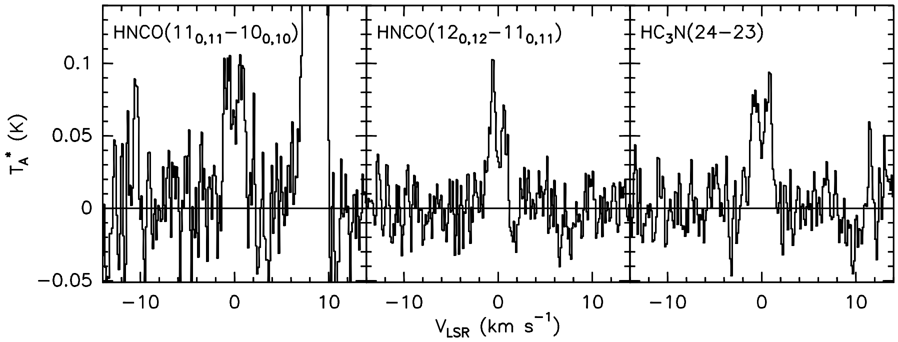

Figure 1. High-resolution spectra of HNCO ($11_{0,11} - 10_{0,10}$), HNCO ($12_{0,12} - 11_{0,11}$), and HC_3N ($24 - 23$) in comet Hale-Bopp. The intensity scale is in antenna temperature units (T_A^*). The lines have characteristic double-peaked line shape expected for optically thin isotropic outgassing. A strong CH_3OH line is present in the left panel at a LSR velocity of 8.5 $km\,s^{-1}$.

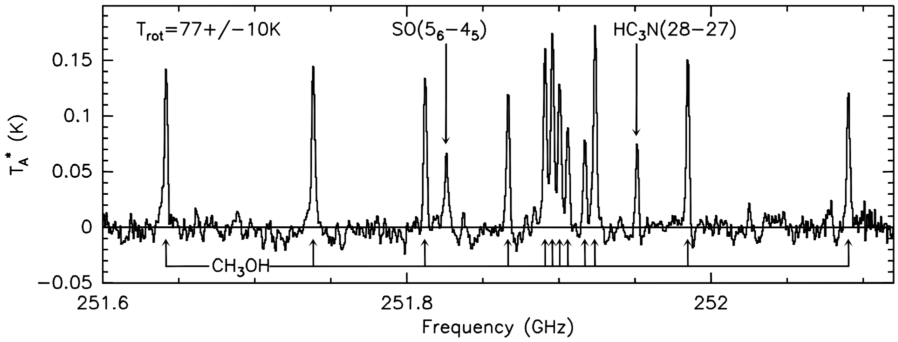

Figure 2. Wideband spectrum of the HC_3N ($28 - 27$) line in comet Hale-Bopp (in the image sideband). A band of 12 methanol lines can also be seen, as well as the ($5_6 - 4_5$) line of SO. The rotational temperature based on the observed intensities of the 252 GHz methanol lines is 77 ± 10 K.

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 β. For a given value of β 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 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.

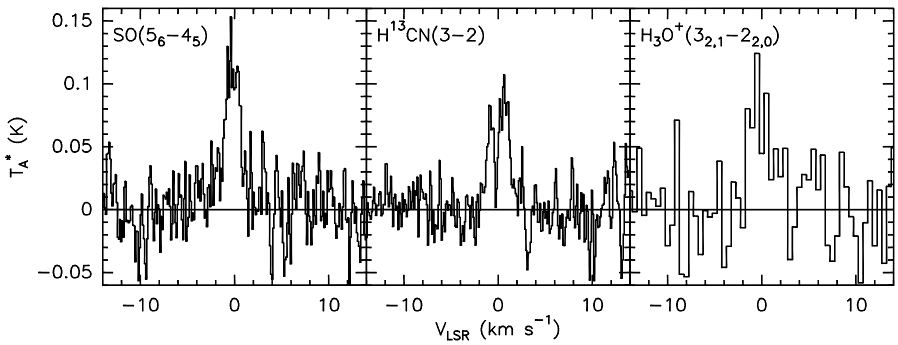

Figure 3. High-resolution spectra of SO ($5_6 - 4_5$), $H^{13}CN$ ($3-2$), and H_3O^+ ($3_2 - 2_2$) in comet Hale-Bopp.

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 ± 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 ± 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 intensity is not at the nucleus position, but $\sim$100,000 km toward the

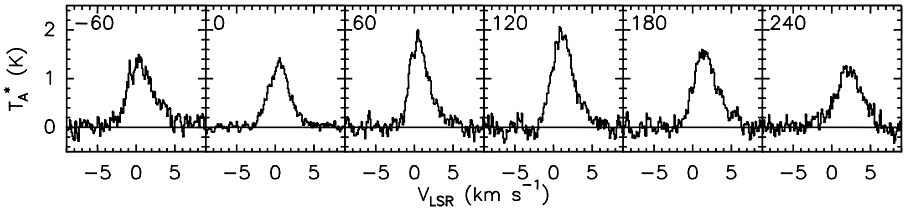

Figure 4. A strip map of HCO^+ emission along the tail. Offsets from the nucleus (in arcsec) are given in the upper-left corner of each panel.

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).

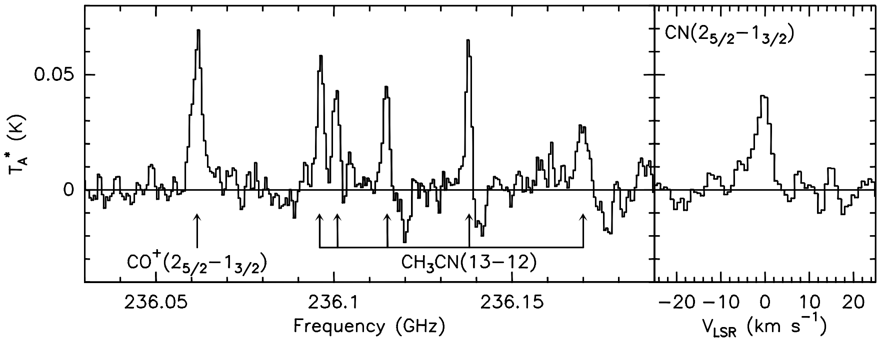

Figure 5. Spectra of CO^+ $(2_{5/2} - 1_{3/2})$ and CN $(2_{5/2} - 1_{3/2})$ in comet Hale-Bopp (left and right panels, respectively). Five lines of CH_3CN from the image sideband can also be seen in the CO^+ spectrum.

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) 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 3σ upper limit for the NaOH production rate derived on Apr. 20-21 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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Address for correspondence:
D.C. Lis, Downs Laboratory of Physics 320-47, California Institute of Technology, Pasadena, CA 91125, USA