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10 February 1997; accepted 3 March 1997

Evolution of the Outgassing of Comet Hale-Bopp (C/1995 O1) from Radio Observations

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Spectra obtained from ground-based radio telescopes show the progressive release of CO, CH₃OH, HCN, H₂O (from OH), H₂S, CS, H₂CO, CH₃CN, and HNC as comet Hale-Bopp (C/1995 O1) approached the sun from 6.9 to 1.4 astronomical units (AU). The more volatile species were relatively more abundant in the coma far from the sun, but there was no direct correlation between overabundance and volatility. Evidence for H₂O sublimation from icy grains was seen beyond 3.5 AU from the sun. The change from a CO-driven coma to an H₂O-driven coma occurred at about 3 AU. The gas outflow velocity and temperature increased as Hale-Bopp approached the sun.

Cometary nuclei are porous bodies consisting of a mixture of ices and refractory grains. Progress made in the identification of cometary volatiles shows that ices of different volatility coexist in the nucleus (1). Although H₂O is the dominant ice and controls cometary activity within 3 AU from the sun, the recent detection of CO in the distant comet P/Schwassmann-Wachmann 1 at millimeter wavelengths (2) suggested that, farther from the sun, cometary activity is

driven by the sublimation of more volatile species. Questions arise as to the physical state and sublimation mechanisms of ices and the relative roles of the various volatiles in the comet's activity. Given the existence of processes causing chemical differentiation within the nucleus, an important issue is whether the molecular abundances measured in the coma near perihelion are representative of the bulk composition of the nucleus. The discovery of Hale-Bopp at heliocentric distance $r_h = 7$ AU (3) offered us the opportunity to address these problems observationally by following the outgassing of this exceptionally bright comet over a wide range of r_h .

Hale-Bopp was observed on a regular basis between August 1995 and late January 1997 with the Nançay telescope, the Institut de Radio Astronomie Millimétrique (IRAM) 30-m telescope (4), and the James Clerk Maxwell Telescope (JCMT) (5) at

decimeter, millimeter, and submillimeter wavelengths, respectively. The OH lines at 18 cm were monitored at Nançay, and observations at IRAM and JCMT focused on rotational lines of parent molecules. The general goals of this campaign were to (i) observe the onset of outgassing of the different species, (ii) monitor their production rates as a function of r_h , and (iii) constrain the kinetic temperature and expansion velocity in the coma and their variation with r_h . Several transitions of the same molecule were observed simultaneously whenever possible to understand the excitation conditions in the coma and to infer the production rates.

Observations at IRAM started in mid-August 1995, when Hale-Bopp was at $r_h = 6.9$ AU (6). Monitoring of OH at Nançay started in December 1995, although preliminary observations had been acquired earlier (7). We detected more than 50 molecular lines, showing the progressive release of nine molecular species (CO, CH₃OH, HCN, OH, H₂S, H₂CO, CS, CH₃CN, and HNC) as the comet approached the sun (Table 1). With the exception of NH₃, OCS, HNCO, and some isotopic species, identified in comet Hyakutake (C/1996 B2) (8), all molecular species detected at radio wavelengths in previous comets were observed in Hale-Bopp at $r_h > 2.4$ AU. A number of species were also observed at other wavelengths. In particular, the first detection of the OH radical was actually obtained with the Hubble Space Telescope (9) 2 weeks before its radio detection. In addition, CO₂, CO, and H₂O were detected at infrared wavelengths by the Infrared Satellite Observatory (10).

Most of the lines in our spectra were blueshifted with respect to the geocentric radial velocity of the comet (Fig. 1). Because the phase angle was always $<20^\circ$, this velocity shift is indicative of anisotropic outgassing with preferred outflow from the sunward side of the nucleus. Coarse mapping of the HCN lines, performed from August to October 1996, showed enhanced outgassing $\sim 45^\circ\text{N}$ from the sun position angle. Beyond $r_h = 3.5$ AU, the OH lines were less blueshifted than the CO lines (Fig. 2A). Although to a lesser extent, the same behavior is observed at $r_h > 4$ AU for the CH₃OH lines. This behavior indicates that some molecular species, such as H₂O and CH₃OH, were partly sublimating from icy grains when observed far from the sun, in contrast to the more volatile CO molecule outgassed mainly from the nucleus. Icy grains of H₂O were detected through their infrared spectral signature at 1.5 and 2.05 μm when Hale-Bopp was at $r_h = 6.8$ AU (11). The low Doppler shifts of the OH and CH₃OH lines (that is, low bulk velocity of

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the H₂O and CH₃OH comae, the bulk velocity being the velocity vector averaged over the whole coma and weighted by the local density) are in agreement with a population of icy grains outflowing at a velocity much lower than the CO velocity and whose whole surface sublimates. Low velocities are expected for large grains and for small grains derived from the fragmentation of larger particles. Enhanced outgassing toward the sun, which may occur for the largest nonisothermal grains, would result in significant spectral blueshifts only moderately affected by the rocket force exerted on the grains. As r_h decreased, the sublimation of grains took place closer to the nucleus, and the collisional coma extended. Molecules released in the collision-dominated coma acquired the bulk average expansion velocity of the gas through conversion of translational energy. The radio observations indicate that sublimating H₂O ice grains were still present in the coma at $r_h = 3.5$ AU. Modeling of sublimation processes in Hale-Bopp (12) showed that the large H₂O production rates observed beyond 3 AU can only be explained by evaporation from icy dust grains. The earlier disappearance of the signature of CH₃OH

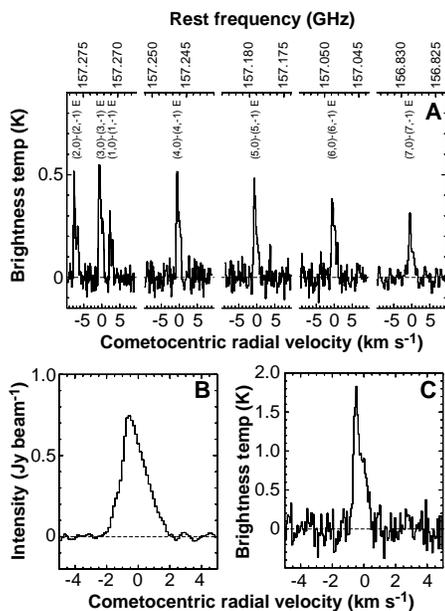


Fig. 1. A selection of radio spectra of Hale-Bopp. **(A)** The 157-GHz group of lines of CH₃OH observed on 10 November 1996 at IRAM. The rotational lines are labeled according to the (J, k) A/E notation for the torsion-rotation levels of CH₃OH (26). **(B)** Average of the 1667- and 1665-MHz lines of the OH radical (scaled to 1667 MHz) observed from 17 to 30 November 1996 at the Nançay radio telescope (1 Jy = 10⁻² W m⁻² Hz⁻¹). **(C)** The J(3-2) CO line at 345 GHz observed on 28 to 29 July 1996 at JCMT. The lower horizontal axis is the radial velocity with respect to the comet rest velocity projected on the line of sight.

sublimating from grains is possibly due to its higher volatility compared to H₂O.

The overall decrease of the CO and CH₃OH Doppler blueshifts, extrapolating toward zero at perihelion (Fig. 2A), indicates a spatial distribution initially restricted to the sunward hemisphere and slowly expanding angularly through the night hemisphere. This may reflect the global increase of the temperature of the nucleus surface, which allowed CO and CH₃OH sublimation over a more extended region as r_h decreased. The systematic blueshift of the OH line observed down to $r_h = 1.4$ AU

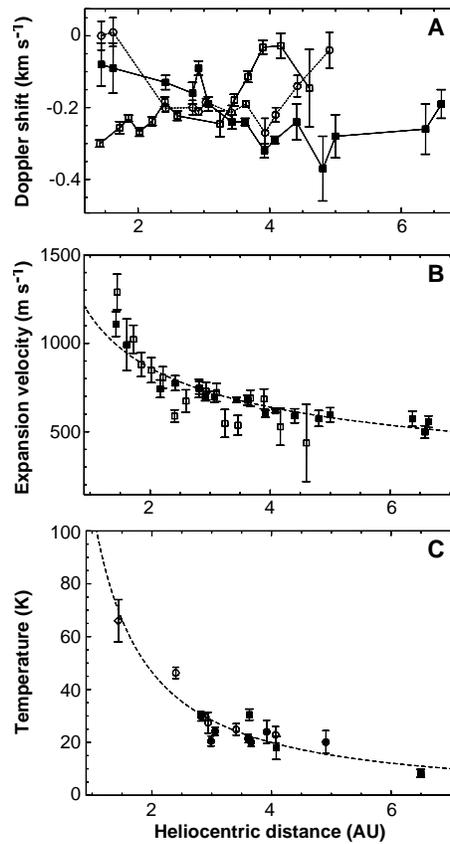


Fig. 2. Evolution of some coma parameters with heliocentric distance r_h . **(A)** Doppler shift of the CO (filled squares), CH₃OH (open circles), and OH (open squares) lines (27). **(B)** Expansion velocity V_{exp} of CO (filled squares) and H₂O (open squares), derived from the line shapes of CO and OH, respectively (27). The dashed line is a power-law fit [$V_{\text{exp}} = (1.16 \pm 0.08)r_h^{(-0.43 \pm 0.02)}$ km s⁻¹] to the CO velocity from 6.6 to 1.4 AU. **(C)** Rotational temperatures derived from the relative intensities of the CO lines (115, 230, 345, and 460 GHz) (filled squares), the CH₃OH 157-GHz multiplet (open circles), and the CH₃OH 304/307-GHz pair (filled circles). These rotational temperatures should be close to the gas kinetic temperature. The value at $r_h = 1.44$ AU (open diamond, far left) is the gas kinetic temperature derived from the rotational temperature of 53 ± 6 K of the 252-GHz CH₃OH lines. The dashed line is the power law fit $T = (109 \pm 35)r_h^{(-1.22 \pm 0.07)}$ K.

would then be due to the H₂O outgassing being more sensitive to diurnal temperature variations than the CO and CH₃OH outgassing (13). An alternative explanation for the low CO Doppler shift at $r_h = 1.4$ AU is a strong contribution of the distributed source of CO as seen in comet P/Halley near perihelion (14).

The line shapes were used to estimate the gas outflow velocity and its evolution with r_h , a necessary parameter for the evaluation of gas production rates from line intensities (Fig. 2B). We derived the CO expansion velocity from the position of the half-peak intensity in the blue wing of the line profile (15). The H₂O outflow velocity was derived from the OH line shapes by the trapezium method (16). The CO velocity follows a variation with r_h close to the commonly used $r_h^{-0.5}$ dependence. The velocity extrapolates to >1 km s⁻¹ at $r_h = 1$ AU, in agreement with previous measurements in other active comets (16, 17). The

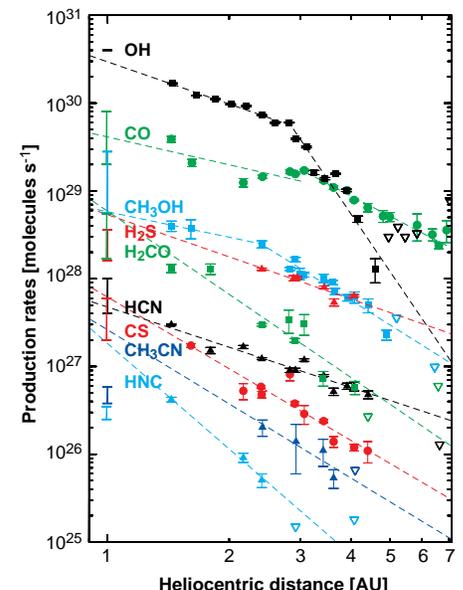


Fig. 3. Evolution of the molecular production rates with heliocentric distance r_h . Filled symbols with error bars correspond to detections; open triangles are upper limits. Exponents of the power-law fits: OH (black squares), -1.60 ± 0.03 ($r_h < 2.8$ AU) and -6.79 ± 0.35 ($r_h > 2.8$ AU); CO (green circles), -1.05 ± 0.13 ($r_h < 3.1$ AU) and -2.39 ± 0.06 ($r_h > 3.1$ AU); CH₃OH (blue squares), -0.96 ± 0.02 ($r_h < 2.4$ AU) and -2.90 ± 0.12 ($r_h > 2.4$ AU); H₂S (red triangles), -1.60 ± 0.14 ; H₂CO (green squares), -3.15 ± 0.18 ; HCN (black triangles), -1.52 ± 0.06 ; CS (red circles), -2.71 ± 0.15 ; CH₃CN (dark blue triangles), -2.8 ± 0.3 ; and HNC (blue triangles), -3.99 ± 0.06 . The vertical bars at $r_h = 1$ AU correspond to the ranges of molecular abundances measured in previous comets near perihelion (7). The scaling was made assuming an OH production rate of 4×10^{30} molecules per second for Hale-Bopp at perihelion.

outflow velocities of H₂O and the other observed species show about the same trends.

Another basic parameter needed to derive production rates from rotational line intensities is the kinetic temperature of the gas. Simultaneous observations of several lines of the same molecule allow one to calculate the rotational temperature of the observed species averaged over the beam. In the inner coma, collisional excitation prevails, and the rotational temperature reflects the kinetic temperature, but in the outer coma, the rotational temperature is determined by radiative excitation. Calculations show that the CO transitions and the CH₃OH lines at 304 to 307 GHz or around 157 GHz act as good thermometers, providing rotational temperatures close to the kinetic temperature within a few kelvin. This is not the case for the HCN lines and the groups of CH₃OH lines around 145, 242, and 252 GHz, whose level populations relax rapidly to fluorescence equilibrium. The gas kinetic temperature increased from about 10 to 65 K from 6.6 to 1.4 AU, roughly as r_h^{-1} (Fig. 2C).

For most species, the models used for converting line intensities into molecular production rates (18) take into account excitation through collisions and fluorescence. The size of the region where the OH 18-cm maser emission is quenched by collisions was constrained with the use of OH data taken at offset positions from the nucleus (19). The measured gas temperature (Fig. 2C) was used to compute the thermal population of the rotational levels in the collision-dominated coma (18). We used Haser density distributions (20) and did not consider the sublimation from grains or the asymmetry of the coma. We assumed that CS was produced by CS₂ and that H₂CO was released from an extended source (21).

At $r_h \geq 4$ AU, CO is the main driver of the activity of Hale-Bopp (Fig. 3). Another significant contributor, not observable at

radio wavelengths, is CO₂ (10). The H₂O, released from grains, and the other volatiles studied here only contribute weakly to the comet's activity at $r_h \geq 4$ AU. As Hale-Bopp approached the sun, molecular species displayed different behaviors in their production rate. At $r_h \geq 2.8$ AU, OH (that is, H₂O) showed a steep variation in production rate roughly as $r_h^{-6.8}$ and a slower increase as $r_h^{-1.6}$ at $r_h < 2.8$ AU. At about 3 AU, the H₂O production rate began to exceed that of CO, marking a change from a CO-driven coma to an H₂O-driven coma. A temporary stagnation is seen for OH between 3.7 and 3.2 AU, which probably reflects the disappearance of H₂O ice grains in the coma and the onset of effective H₂O sublimation from the nucleus, as expected from modeling (22). The heliocentric total visual magnitudes also show a plateau at the same r_h 's, which may be related to the change of regime from dust dragged by CO to dust dragged by H₂O. The heliocentric variation of the H₂O production rate observed between 1.4 and 2.8 AU is close to the r_h^{-2} dependence predicted by heat flow models at these distances (23).

After H₂CO (24), CS, CH₃CN, and CH₃OH were first observed in the comet, their production rates rose rapidly, roughly as r_h^{-3} . The production rates of CO, H₂S, and HCN increased more slowly, with slopes between $r_h^{-1.5}$ and $r_h^{-2.4}$. Our marginal detections and upper limits suggest that the onset of outgassing of CH₃OH and HCN was more rapid than their subsequent evolution. As Hale-Bopp approached 3 AU, the evolution of the outgassing of some species changed, as for H₂O. The CO production rate stagnated and then rose again at $r_h \sim 2$ AU. The CH₃OH production rate increased more slowly. The rate of HNC production showed a steep evolution as r_h^{-4} since its detection at $r_h = 2.4$ AU (Table 1).

We would expect the more volatile species to be relatively more abundant in the coma far from the sun. Although there are differences with molecular abundances

measured in other comets at $r_h \sim 1$ AU, there is no simple correlation between overabundance and volatility (defined by the sublimation temperature of the pure ices). The most volatile species, CO and H₂S, are indeed overabundant in Hale-Bopp at 4 AU, but HCN, which is also overabundant, has the same sublimation temperature as CH₃CN and CH₃OH, both found with normal ratios at this distance. These differences presumably reflect the number of physicochemical processes taking place inside a comet nucleus as a result of solar heating, causing chemical differentiation. A thermodynamic model was used to simulate the evolution of the H₂O and CO production rates in Hale-Bopp (12). When H₂O ice is amorphous, this model is able to explain the CO production rate measured at $r_h > 3$ AU with a CO source underneath the comet's surface. This model predicts the stagnation seen at 3 AU, due to the increasing depth of the CO sublimation front. It also predicted the increase in CO seen at $r_h \sim 2$ AU, due to the decrease of the depth of CO sublimation resulting from surface erosion caused by H₂O sublimation.

As r_h decreased, the relative molecular production rates approached those found in other comets near 1 AU (1). This indicates that, in terms of chemical composition, Hale-Bopp is a typical comet. The notable exception is HNC. This unstable species was detected in Hyakutake at $r_h = 1$ AU (25) with a relative abundance to HCN of 6%. It was argued that the strong similarity of the HNC/HCN ratio in comets to those observed in warm quiescent molecular clouds suggests that cometary nuclei are composed of relatively unprocessed molecular ices. This ratio was less than 2% in Hale-Bopp at 2.9 AU and increased up to 20% at 1.4 AU. Although little is known about the thermodynamic properties of HNC ices, these strong variations cast doubt on the true value of the HNC/HCN ratio in cometary nuclei. The similarity of the heliocentric evolution of the HNC outgassing with that of H₂CO (24), known to be produced from an extended source in the coma rather than from the nucleus (21), might argue against a nuclear origin.

Table 1. Observed molecular species with approximate dates of the first unambiguous detection with corresponding r_h and the main frequencies at which each was observed in the present work.

Species	First detection			Main frequencies observed (GHz)
	Date	r_h (AU)	Ref.	
CO	September 1995	6.9	(6, 22)	115.3, 230.5, 345.8, 461.0
CH ₃ OH	March 1996	4.9	(28)	97,* 145,* 157,* 242,* 252,* 304.2, 307.2
HCN	April 1996	4.8	(29)	88.6, 265.9, 354.5
OH	April 1996	4.7	(30)	1.612, 1.665, 1.667, 1.720
H ₂ S	May 1996	4.3	(31)	168.7
H ₂ CO	June 1996	4.1	(32)	218.2, 225.7, 351.8
CS	June 1996	4.1	(32)	98.0, 147.0, 244.9, 342.9
CH ₃ CN	August 1996	3.4	(33)	147.1*
HNC	November 1996	2.4	(34)	90.6, 272.0

*Multiple transitions observed.

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4. The half-power beam width (HPBW) of the IRAM antenna is 10 arc sec at 230 GHz and 26 arc sec at 89 GHz. Most of the spectra were acquired at a spectral resolution of 20 to 40 kHz, corresponding to

- velocities of 0.026 to 0.052 km s⁻¹ at 230 GHz. Whenever possible, a frequency-switching mode was used.
- The HPBW of the JCMT antenna is 14 arc sec at 345 GHz. Most data were obtained in the 300- to 370-GHz window with a spectral resolution of 95 kHz, in the frequency-switching mode.
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 - Observations with the Nançay radio telescope (right ascension × declination of the HPBW was 3.5 arc min × 19 arc min) were undertaken with the technique previously used for comet P/Halley and other comets [E. Gérard, D. Bockelée-Morvan, G. Bourgois, P. Colom, J. Crovisier, *Astron. Astrophys. Suppl. Ser.* **77**, 278 (1989)].
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 - The quenching radius r_q was estimated to have been $\sim 2.6 \times 10^5$ km in October and November 1996 at $r_h = 2.2$ to 2.7 AU, determined using the center exposure and the average east-west offset positions at 7 and 14 arc min, as in comet Hyakutake [E. Gérard *et al.*, in preparation]; the quenching was modeled according to $r_q = r_{q0} Q_{OH}^{0.5}$ [F. P. Schloerb, *Astron. Astrophys. J.* **332**, 524 (1988)], with $r_{q0} = 40,000$ km, r_h in astronomical units, and the OH production rate Q_{OH} in units of 10^{29} s⁻¹. We used the OH lifetime computed at solar minimum [S. A. Budzien, M. C. Festou, P. D. Feldman, *Icarus* **107**, 164 (1994)].
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13 February 1997; accepted 6 March 1997

The Spectrum and Spatial Distribution of Cyanogen in Comet Hale-Bopp (C/1995 O1) at Large Heliocentric Distance

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Optical spectra of comet Hale-Bopp (C/1995 O1) at a heliocentric distance of 6.45 astronomical units showed emission from cyanogen gas. The spatial distribution of cyanogen was considerably more diffuse and extended compared to the spatial profile of the dust or grains which were sharply peaked near the center. This behavior is consistent with comets at smaller heliocentric distances suggesting the same or a similar formation mechanism. A cyanogen gas production rate of $(1.2 \pm 0.3) \times 10^{26}$ molecules per second was derived. A model band profile derived from fluorescence equilibrium calculations for the comet's heliocentric velocity and distance agrees with the observed band profile.

Comet Hale-Bopp (C/1995 O1) was discovered on 23 July 1995 at an integrated visual magnitude of ~ 11 (1) and at a heliocentric distance, r_h , of 7 astronomical units (AU) (2). The discovery of a luminous periodic comet at such a large distance from the sun initiated observations at optical and radio wavelengths to understand the physical and chemical processes occurring in the nucleus and coma which are not available from observations at smaller r_h . In particular, Fitzsimmons and Cartwright (3) detected emission from the CN (0-0) band in Hale-Bopp's coma at $r_h = 6.82$ AU; the second most distant reported detection for a comet (4, 5).

Our observations of Hale-Bopp were ob-

tained on 13.1 October 1995 universal time (UT) ($r_h = 6.45$ AU; 6.64 AU from Earth) with the 4.5-m Multiple Mirror Telescope and the blue channel charge-coupled device spectrograph (6). We obtained two 20-min exposures of Hale-Bopp with the spectrograph slit centered on the nucleus throughout the observation and oriented along the parallactic angle of 29° to minimize any loss of light due to atmospheric refraction. The position angle of the sun on the plane of the sky was 270° so that the slit was oriented nearly orthogonal to sun-tail direction on the sky. The spectrum of a solar analog star (van Bueren 64) was obtained to remove the reflected solar spectrum from the comet spectrum. The first comet exposure was heavily contaminated by background stars and was discarded.

The data were reduced and processed using standard procedures (7). Because any gas coma of Hale-Bopp is expected to be quite extended and probably even extends beyond the bounds of our short slit, sky subtraction was accomplished by first inter-

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