New results on the composition of comets

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0.1 Introduction

Comets are likely the most pristine material surviving from the origin of the Solar System. Because they accreted in the coldest regions of the solar nebula, an important question is whether cometary nuclei retained the molecular composition inherited from the protosolar cloud, as originally proposed by Greenberg [17] or are a product of solar nebula chemistry ([23]). In the former case, the origin of comets could be searched in the cold stages of the protosolar cloud and molecular abundances of grain mantles as well as the nature of refractories in this cloud may be similar to those in cometary nuclei. Alternatively, the formation region of comets may have undergone sufficient heating to sublimate the most volatile species of the icy mantles ([37]). The heating could have been even more substantial and cometary ices may be a second generation of ices which recondensed onto the cold grains in equilibrium with the nebular gas ([24]). A good knowledge of the cometary composition should provide clues to these different scenarios. The challenge is not only a better understanding of the origin of cometary material, but strong constraints on the evolution of matter at the stages from interstellar clouds to planetary systems may be expected.

We will review here progresses made recently on the nature of cometary ices and refractories, thanks the spectacular apparitions of comets C/1996 B2 (Hyakutake) and C/1995 O1 (Hale-Bopp) . Discovered in January 1996, Hyakutake is a long-period comet who made a very close approach to Earth at the end of March 1996 at only 0.10 AU where its total visual magnitude decreased below 0. Hale-Bopp , also a long-period comet, was discovered exceptionally active in July 1995 at 7 AU from the Sun. This extraordinary activity, at a distance where the sublimation of water is inefficient, was found to be due to the vaporization

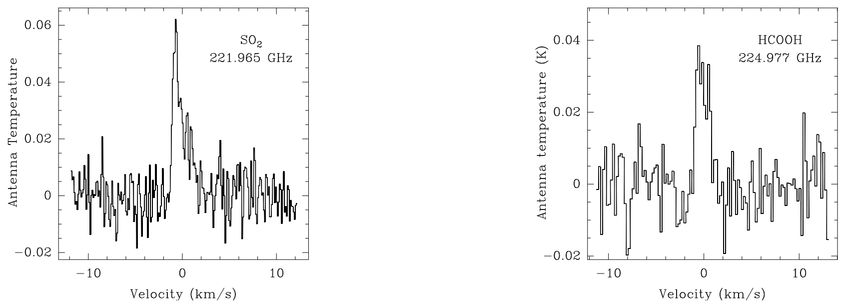

Figure 1: Detection of SO_2 ($11_{1,11}$–$10_{0,10}$) and HCOOH (blend of $10_{5,6}$– $9_{5,5}$ and $10_{5,5}$–$9_{5,4}$) in comet Hale-Bopp with the IRAM Plateau de Bure interferometer on March 18–21 and March 20–21 1997, respectively ([36], [35]).

of super-volatiles, mainly CO ([20], [4], [3]) and CO_2 ([11], [12]). Around perihelion at 0.9 AU from the Sun, on April 1, 1997, the gaseous production rate exceeded 10 times that of P/Halley at the same heliocentric distance and the visual magnitude decreased down to -2.

0.2 New molecular species

The most direct method for probing cometary ices is the observation in the coma of the so-called parent molecules which directly outgass from the nucleus. Because most parent molecules have weak spectral signatures in the UV and visible, they have to be searched for in the infrared and microwave domains through their vibrational bands or rotational lines.

Prior to comets Hyakutake and Hale-Bopp, our knowledge of cometary volatiles was limited to detections of H_2O, CO, CO_2, CH_3OH, H_2CO, HCN, H_2S and S_2 (see e.g. [10], [30]). NH_3 was marginally observed in comet C/1983 H1 (IRAS-Araki-Alcock) and its abundance was estimated in several comets from the observation of its photodissociation products. CS_2 was inferred from UV observations of the CS radical. If we exclude isotopomers, the number of identified parent species has now been multiplied by more than two. Most new species were detected in the millimetre or submillimetre range. Identifications in the infrared benefited from the high spectral resolution provided by echelle spectrographs.

Several new nitrogen-bearing species were detected using microwave spectroscopy. HNC, CH_3CN and HNCO were first identified in comet Hyakutake and extensively observed in comet Hale-Bopp. HC_3N and formamide NH_2CHO were identified in Hale-Bopp. NH_3 was definitely identified at centimetre wavelengths in both comets.

Table 1: Molecular abundances in comet Hale-Bopp near perihelion [a]

molecule	abundance[b]	method	comments	references
H_2O	100	IR		[12], IAUC 6604
CO	20	radio, IR, UV		[3]
CO_2	6[c]	IR		[11], [12]
CH_4	~ 1	IR		[27], IAUC 6573
C_2H_2	~ 0.5	IR		[27], IAUC 6573
C_2H_6	~ 0.5	IR		[27], IAUC 6573
CH_3OH	2	radio, IR		[3]
H_2CO	~ 1[d]	radio	extended	[3]
HCOOH	0.05	radio		IAUC 6599
$HCOOCH_3$	0.05	radio		IAUC 6645
NH_3	0.6	radio		[2]
HCN	0.2	radio, IR		[3]
HNCO	0.1	radio		IAUC 6566
HNC	0.03	radio		[3]
CH_3CN	0.02	radio		[3]
HC_3N	0.02	radio		IAUC 6566
NH_2CHO	0.01	radio		IAUC 6614
H_2S	1.6	radio		[3]
SO	0.6	radio	from SO_2 ?	IAUC 6573
CS	0.2	radio, UV	from CS_2 ?	[3]
SO_2	0.15	radio		IAUC 6591
OCS	0.5	radio, IR		IAUC 6573, 6682
H_2CS	0.02	radio		IAUC 6607
S_2	0.005[a]	UV		[33]

[a] The abundance given for S_2 is that measured in Hyakutake ([33]). S_2 has not been detected in Hale-Bopp.
[b] abundances relative to water. Most values are preliminary estimates. Except for CO_2, H_2O and hydrocarbons, they are derived from radio measurements.
[c] assuming the CO_2/CO abundance ratio measured at 3 AU from the Sun ([12]).
[d] Abundance in the coma. Abundance in the nucleus may be much smaller.

A number of sulfur-bearing species were also observed for the first time. Surprising were the millimetre detections in Hale-Bopp of SO and SO_2 (Fig. 1), for which sensitive upper limits were obtained in the UV in other comets (but this might be due to ill-known UV excitation of these molecules rather than to an abundance diversity in comets). OCS and H_2CS were directly observed. The close approach to Earth of Hyakutake allowed the UV detection of the short-lived species S_2 ([33]), previously seen in IRAS-Araki-Alcock.

HCOOH (Fig. 1) and $HCOOCH_3$ complete the inventory of new parent species detected in Hale-Bopp in the microwave. Observations in the infrared allowed the discoveries of CH_4, C_2H_6 ([28]) and C_2H_2 ([7]) in Hyakutake.

Table 1 gives volatile abundances measured in comet Hale-Bopp near 1 AU from the Sun, where the activity is driven by the sublimation of water ice. Abundances in Hyakutake, as reviewed in [5], were similar. These abundances, especially those of the more volatile species, may not reflect exactly the original composition of nuclear ices due to the number of chemical fractionation processes occurring inside the nucleus upon solar heating. As a matter of fact, the coma of comet Hale-Bopp farther from the Sun showed quite a different composition with the more volatile species being relatively more abundant ([3]).

0.3 Cometary silicates

The composition of cometary grains was first addressed by the dust analysers on the Giotto and Vega space probes. Two different chemical phases were found: an organic phase composed of carbon, hydrogen, oxygen and nitrogen (called CHON) contributing to 30 % of the total mass of the measured particles and a Mg-rich silicate phase [19]. The discovery of a bi-modal grain composition demonstrated the pristine nature of the dust of P/Halley.

Spectra of the 10 μm silicate emission feature in P/Halley and other comets allowed to precise the nature of the silicates . Some of them showed a prominent narrow 11.25 μm peak attributed to crystalline olivine and a broad maximum at 9.8 μm indicative of amorphous silicates ([22]). Ground-based observations of Hale-Bopp showed distinctly shoulders at 11.9 and 9.2 μm, associated also to crystalline and glassy silicates, respectively ([21]).

The observation of the full 7–45 μm spectral range in Hale-Bopp by ISO brought definite insights on the mineralogy of its silicates ([12]). Additional emission features at 16, 19.5, 23.5, 27.5 and 33.5 μm were observed (Fig. 2). They all correspond to the signature of crystalline olivine and are best matched by a Mg-rich olivine (like forsterite Mg_2SiO_4). Hanner ([21]) shows that the relative strength of 11.25 μm feature implies that about 20 % of the silicates are in the form of crystalline olivine, the most abundant fraction being glassy olivine or pyroxene.

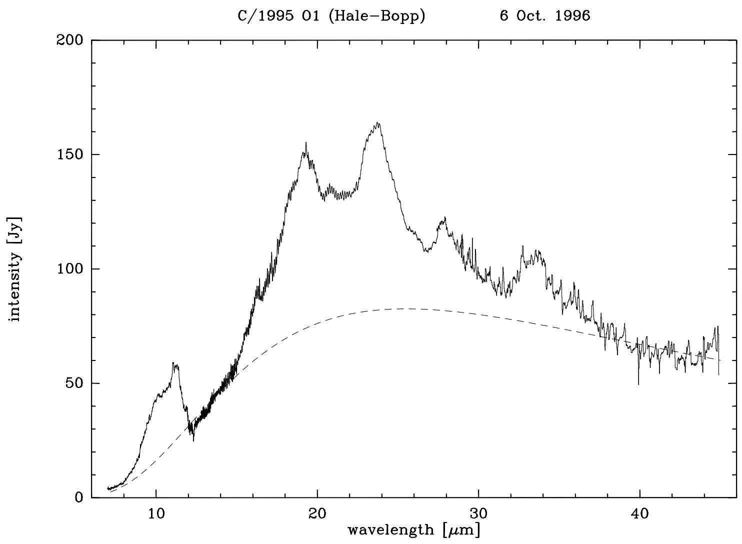

Figure 2: The 7 to 45 μm spectrum of Hale-Bopp observed with the SWS on ISO on 6 October 1996 ([12]). The emission features correspond to thermal emission of Mg-rich crystalline olivine. The dotted line shows a black-body curve fitted to 7.5 and 13 to 15 μm.

0.4 Discussion

Comets may have diverse compositions betraying different origins. Indeed, A'Hearn et al. ([1]), from broad-band spectrophotometry of cometary radicals, identified a class of carbon-depleted comets that seems to coincide with Jupiter-family comets. These latters are short-period comets supposed to come from the Kuiper belt , whereas Halley-type and long-period comets are coming from the Oort cloud . Direct information on parent molecules, however, are still sparse, and the best documented cases — P/Halley, Hyakutake and Hale-Bopp — are for Oort cloud comets only.

Mumma et al. ([30]) extensively discussed the composition of comets in terms of the origin of cometary material. They pointed out that the CH_4 to CO mixing ratio, the high HCN and NH_3 abundances and the presence of H_2CO, CH_3OH and other organics do not support formation in the solar nebula. By contrast, the strong analogies between abundances in cometary and in interstellar ices may suggest origin in the protosolar cloud. ISO observations of new solid state features towards protostellar objects allowed to extend the analogy found for H_2O, CH_3OH and CO to CO_2, CH_4 and OCS ([34], [14]). HNCO and NH_2CHO might be linked to the mysterious "XCN" species observed in interstellar ices.

The new species detected in comets Hyakutake and Hale-Bopp strengthen the case for an interstellar origin. Most of them are found in galactic hot cores which are parts of giant molecular clouds where high-mass stars are forming. These clouds are rich in saturated molecules and contain also complex oxygen-bearing molecules, which are difficult to form in pure gas-phase chemical reaction schemes. Therefore, they are thought to have been formed in an earlier cold phase by gas/grain processes, before being evaporated. According to modelling ([9]), H_2CO, CH_3OH, HCOOH, HNCO and NH_2CHO are readily formed by hydrogenation of CO and further atom addition at the surface of the grains. C_2H_2 can form by ion-molecules reaction in the gas phase and accrete with a large abundance on grains in cold clouds ([8]). Predicted C_2H_2/CO abundances are high, as observed in comets. H-atom addition to accreted C_2H_2 leads to C_2H_6. Although never observed in the interstellar medium (ISM), the presence of abundant ethane in comets is thus naturally explained by interstellar gas/grain chemistry ([28]).

It has been argued that the interstellar nature of cometary volatiles is also supported by the presence of HNC ([18]). The observed high HNC/HCN mixing ratio (6 % in Hyakutake, 2 to 20 % in Hale-Bopp) cannot be explained by thermal equilibrium reactions that presumably occurred in the solar nebula, but is in the range of ratios observed in quiescent molecular clouds. However, the variation of HNC/HCN with heliocentric distance seen in comet Hale-Bopp questions the effective HNC abundance in the nucleus ([3]).

There are other key indicators for an interstellar origin of cometary volatiles. As discussed elsewhere in this conference ([16]), the high D/H ratios in water (3×10^{-4}, [13], [6], [25]) and in HCN ($\sim 10^{-3}$, [26]) can only be explained by ion-molecule isotopic exchanges in the ISM. The ortho/para ratio in water attests to a low temperature region ([29], [12]). We have also several indirect evidences that water ice is amorphous ([15]), as expected for formation in cold environments. On the other hand, the presence of crystalline silicates in some comets may call into question that comets directly accreted from unprocessed interstellar grains. Indeed, the silicates in the ISM essentially appear to be amorphous. Conversion of this material to the crystalline form requires restructuring the lattice, which can be done by heating the grains. Such a processing has certainly taken place in the inner solar nebula. In this case, this would indicate that comets formed in a region where grains originating from the inner solar nebula were present. However, this scenario is difficult to reconcile with the high deuterium enrichment which suggests that comets formed in the non-turbulent region of the solar nebula ([6], [16]).

Alternatively, crystalline silicates have been found in dust shells around evolved stars ([32]). At least a fraction of interstellar silicates should be crystalline. Mg-rich crystalline silicates were also found in circumstellar disks of young main-sequence stars ([31]). There is thus a definite link between protoplanetary disks and the primordial material of our Solar System found in comets.

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