Planetary Systems in the Universe - Observation, Formation and Evolution
Proceedings IAU Symposium No. 202,
Alan Penny, Pawel Artymowicz, Anne-Marie Lagrange, & Sara Russell, eds.

Molecular Observations of Comets: Constraints for Planetary System Formation

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Abstract. We review our knowledge of the composition of cometary volatiles in the light of recent observations of comets C/1996 B2 (Hyakutake) and C/1995 O1 (Hale-Bopp) and examine how this could constrain models of planetary system formation.

The recent observations of comets C/1996 B2 (Hyakutake) and C/1995 O1 (Hale-Bopp), especially at radio wavelengths, led to the detection of many new cometary molecules, thus allowing us to complement our inventory of the composition of cometary volatiles (Bockelée-Morvan 1997, Lis et al. 1997, Bockelée-Morvan et al. 2000 and references therein). A summary of the volatile abundances observed in these two comets is given in Table 1. In addition to abundant species (H_2O, CO, CO_2, CH_3OH, H_2CO...), this inventory now includes hydrocarbons, nitrogen compounds NH_3, HCN, HNC, HNCO, HC_3N, CH_3CN), sulphur compounds (H_2S, CS_2, SO, SO_2, OCS ...), and fairly complex organic molecules found at the trace level, such as formic acid (HCOOH), CH_3CHO, NH_2CHO, $HCOOCH_3$. Isotopic ratios, especially D/H in water and HCN, were evaluated (Bockelée-Morvan et al. 1998; Meier et al. 1998a, 1998b). Several species were also searched for unsuccessfully, some of them with stringent upper limits: ethanol, ketene (CH_2CO), methanimine (CH_2NH), HC_5N, and many others (a summary of these unpublished results is given in Table 2).

These results provide clues to the composition of the primitive Solar Nebula and give important constraints for models of planetary formation. For the most abundant species (H_2O, CO, CO_2, CH_3OH, H_2CO, CH_4, OCS, nitriles X–CN), there is a strong analogy between cometary volatiles and interstellar ices (such as those observed in the infrared by ISO towards deeply embedded protostars

Table 1. Relative production rates of molecules observed in comets C/1996 B2 (Hyakutake) and C/1995 O1 (Hale-Bopp) at $r_h \approx 1$ AU.

Molecule	[a]	[b]	C/1996 B2	C/1995 O1	remark
H_2O	IR	> 5	100	100	
CO	R IR UV	> 5	6–30	23	extended[c]
CO_2	IR	2	–	20[d]	
CH_4	IR	2	0.7	0.6	
C_2H_2	IR	–	≈ 0.5	0.1	
C_2H_6	IR	2	0.4	0.3	
CH_3OH	R IR	> 5	2	2.4	
H_2CO	R IR	> 5	0.2–1	1.1	extended[e]
HCOOH	R	–	–	0.08	
CH_3CHO	R	–	–	0.02	
$HCOOCH_3$	R	–	–	0.08	
NH_3	R IR	1?	0.5	0.7	
HCN	R IR	> 5	0.1	0.25	
HNCO	R	–	0.07	0.10	
HNC	R	1	0.01	0.04	extended
CH_3CN	R	–	0.01	0.02	
HC_3N	R	–	–	0.02	
NH_2CHO	R	–	–	0.015	
H_2S	R	5	0.8	1.5	
OCS	R IR	–	0.1	0.4	extended
SO	R	–	–	0.3	extended
CS_2	(R) (UV)	> 5	0.1	0.2	from CS[f]
SO_2	R	–	–	0.2	
H_2CS	R	–	–	0.02	
S_2	UV	2	0.005	–	

[a] technique of observation (R = radio); [b] number of detections in other comets; [c] abundance given for *nuclear* + *extended* source; [d] measured at $r_h = 2.9$ AU; [e] abundance given for *extended* source; [f] CS_2 abundance inferred from CS. Detailed references may be found in Bockelée-Morvan et al. 2000.

(Ehrenfreund & Schutte 2000). This comparison cannot be extended to trace species because of the lack of sensitivity of infrared observations. A quantitative comparison was also made with the abundances observed by radio spectroscopy in hot molecular cores and bipolar flows (Bockelée-Morvan et al. 2000). There is a very good agreement for the N-bearing and CHO-bearing species. There is less agreement for the S-bearing species, an expected result since the abundances of sulphur species in hot cores and bipolar flows may be affected by a rapid gas-phase chemistry in the post-evaporation phase.

Table 2. Upper limits on the relative production rates of undetected molecules in comets (radio observations).

Molecule	line [GHz]	limit[a]	telescope	comet
H_2O_2	362.156	< 0.04	CSO	Hyakutake
CH_3CCH	222.167	< 0.045	IRAM PdB	Hale-Bopp
CH_2CO	220.178	< 0.032	IRAM 30-m	Hale-Bopp
C_2H_5OH	235.983	< 0.05	IRAM 30-m	Hale-Bopp
CH_3OCH_3	several	< 0.45	IRAM 30-m	Hale-Bopp
CH_3COOH	several	[b]		Hale-Bopp
glycine	several	< 0.5	IRAM 30-m	Hale-Bopp
HC_5N	several	< 0.003	IRAM 30-m	Hale-Bopp
CH_2NH	226.548	< 0.032	IRAM 30-m	Hale-Bopp
CH_3SH	radio	[b]		Hale-Bopp
NaOH	251.226	< 0.0003	CSO	Hale-Bopp
NaCl	260.223	< 0.0008	CSO	Hale-Bopp

[a] relative to water = 100. [b] limit not yet evaluated

The correlations between molecular abundances ranging over several orders of magnitude reinforce the similarity between interstellar and cometary ices. There is now strong evidence that cometary ices were formed to a large extent by the same low temperature non-equilibrium processes which produce interstellar ices: grain surface reactions, condensation of products of ion-molecule reactions, UV processing. But is there a direct link between interstellar and cometary ices? In the inner part of the protoplanetary disc, the high temperature led to a complete volatilization (up to atomisation) of the grains and initiated a specific solar nebula thermochemistry. Assessing to which extent nebular chemistry and additional processes, such as accretion shocks and radial mixing in the nebula, have also contributed to cometary ice composition will need further studies, but the similarities with interstellar ices shown by the present data clearly set a limit to their relative importance.

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