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Making a comet nucleus

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Abstract. The chemical composition of a comet nucleus can be very strictly constrained by combining the latest results on: the core-mantle interstellar dust model, the solar system abundances of the elements, the space observed composition of the dust of comet Halley, and the latest data on the volatile molecules of comet comae. The distribution of the components in the comet nucleus fall naturally into two basic categories – refractories and volatiles. The refractory components are tightly constrained to consist of about 26% of the mass of a comet as silicates (a generic term for combinations of the elements Si, Mg, Fe), 23% complex organic refractory material (dominated by carbon), and about 9% in the form of extremely small (attogram) carbonaceous/large molecule (PAH) particles. The remaining atoms are in an H₂O dominated mixture containing of the order of 2 – 3% each of CO, CO₂, CH₃OH plus other simple molecules. The H₂O abundance itself is very strictly limited to $\sim 30\%$ of the total mass of a comet – not much more nor much less. The refractory to volatile (dust to gas) ratio is about 1:1, while the dust to H₂O ratio is $\approx 2 : 1$. The maximum mean density of a fully packed nucleus would be $\approx 1.65 \text{ g cm}^{-3}$. The morphological structure of the component materials, following the interstellar dust into the final stage of the presolar cloud contraction, is as tenth micron silicate cores with organic refractory inner mantles and outer mantles of “ices” with each grain containing many thousands of the attogram carbonaceous/large molecule particles embedded in the icy and outer organic fraction.

Key words: comets: general – comets: individual: P/Halley – ISM: dust – ISM: molecules – ISM: abundances

1. Introduction

The chemical composition of a comet nucleus has often been described as a dirty snow ball. This originated with the pioneering work of Whipple (1950, 1951) who suggested almost 50 years ago that a comet nucleus is a well defined “solid” object dominated by water ice. However, while this term is still being used today it does not provide an operationally adequate basis

for understanding either the evolution of comet nuclei or the coma dust and molecules. For example, it could not anticipate the major “surprises” discovered by the space missions to comet Halley. Nevertheless, Whipple anticipated two major features of our current perception. One was that he believed that “the relative abundance of the elements in comets should be typical of the universe at large, with the limitation that elements not freezing or forming compounds should be rare or absent”.

It is indeed commonly assumed that comet nuclei, as the most primitive solar system objects, have an atomic composition which is well represented by solar system abundances of condensable elements (excluding hydrogen and helium, of course) and they have often been compared with carbonaceous chondrites, though the latter are certainly less primitive. Whipple also suggested that “... the meteoric materials should constitute about one-third or less the mass of cometary nuclei, the other two-thirds being made up largely of the hydrides of C, N and O.” In fact these latter resembled the “dirty ice” model of interstellar dust proposed by Van de Hulst (1949). We shall see that such a comet nucleus would contain more ice than can be accommodated within the solar system abundance constraints. In addition, until about 15 years ago there was a puzzling lack of carbon relative to oxygen in the coma (volatile) molecules (Delsemme 1982). By coincidence, in that same volume, Greenberg (1982) published a nucleus chemical composition based on the silicate core-organic refractory mantle interstellar dust model which automatically accounted for the missing carbon as being contained in the complex organic molecules resulting from ultraviolet photoprocessing of the interstellar ices which, rather than contributing much to the coma gas molecules, were a major contributor to the dust. This component in fact constituted a major fraction of the nucleus mass, about equal to the silicates (Whipple’s meteorics), based on the interstellar dust model. In that first quantitative derivation of how the atoms are distributed in the molecules of the comet no attempt was made, a priori, to fit comet data. Rather, the construction was a purely inductive one in that it was taken as given that in the final stage of presolar cloud contraction the interstellar dust as it was then modeled and, consistent with solar system abundances, would contain all the condensable atoms and would aggregate without further modification into comet nuclei. This first purely interstellar dust model, primitive and naive as it was, actually worked sur-

prisingly well in predicting the major surprises resulting from the space missions to comet Halley – the large abundance of very small particles and the organics as a major fraction of the dust (Greenberg 1986; McDonnell et al. 1986; Kissel et al. 1986a, b). Further analysis of the data showed that the organic (CHON) molecules had, on the average, a higher initial energy than the silicate ions which led Krueger & Kissel (1987) to infer a core-mantle structure of the dust particles. Thus according to Jessberger & Kissel (1991) “The existence of the previously postulated (Greenberg 1982) core-mantle grains seems to be substantiated by data”. The aggregated interstellar dust model has also served as a basis for further theoretical extensions in terms of morphological properties of porous nuclei (Greenberg, Mizutani & Yamamoto 1995; Tancredi et al. 1994; Haruyama et al. 1993) and comet dust (Greenberg & Hage 1990; Li & Greenberg 1998) in which the basic units are the tenth micron interstellar dust grains.

In principle, if we could follow an interstellar cloud through its entire collapse phase to form a solar system and, in particular comets, this approach should be reliable. But our information on interstellar dust stops short of this final phase, being limited to observations and theories which take us up to dense molecular clouds and to post-stellar formation regions but never in between. The alternative, to go backwards from observations of the coma and tail of a comet to derive the originating nucleus is also limited because of the complex interactions not only at the nucleus surface but also in the coma. Although, using the latter now seems to offer some advantages because of the great abundance of new data on the molecules and dust in the comet coma, there is also a clear correspondence between dust mantle molecules and coma molecules which suggests that it may be useful to compare both approaches. In any case it seems appropriate to assume that at most only the volatile components of the interstellar dust may have partially evaporated before the comet nucleus formed and even this may not have occurred.

In this paper I shall demonstrate how constructing a comet nucleus by combining the interstellar dust refractories with coma volatiles leads to a remarkably well defined set of molecular compositions. For comparison I will also derive a comet composition using a purely interstellar dust model; i.e., using data on the dust ices (rather than coma molecules) along with refractories. The key constraints in both constructions are the assumption of solar system abundances and the core-mantle interstellar dust model.

2. Solar system abundances

The relative abundances of the elements are a subject of major importance in understanding the formation of the solar system. Considerable effort has been devoted to trying to settle on an agreed set of abundances. In Table 1 I show some typical examples of the abundances of the major condensable species obtained over the past 15 years. It is immediately recognized that the major pattern has not changed which gives us some confidence in the results. The most recent tabulation is represented by the last column with two alternative values for the carbon

Table 1. Relative (solar system) abundances of the most common elements.

Element	1	2	3	4
H	1	1	1	1
He	0.068	0.081	0.079	0.098
C	4.17(-4)	4.45(-4)	4.90(-4)	4.44(-4)*
N	0.87(-4)	0.91(-4)	0.98(-4)	0.93(-4)
O	6.92(-4)	7.40(-4)	8.13(-4)	7.44(-4)
Mg	0.399(-4)	0.396(-4)	0.380(-4)	0.38(-4)
Si	0.376(-4)	0.368(-4)	0.355(-4)	0.355(-4)
S	0.188(-4)	0.189(-4)	0.162(-4)	0.214(-4)
Fe	0.338(-4)	0.331(-4)	0.467(-4)	0.316(-4)

(1) A.G.W. Cameron (1982), in “Elements and Nuclidic Abundances in the Solar System”, ed. C. Barnes, R.N. Clayton & D.N. Schram (Cambridge Univ. Press), 23;

(2) E. Anders & Mitsuru Ebihara (1982), *Geochimica & Cosmochimica Acta* 46, 2363;

(3) N. Grevesse (1984), *Physica Scripta* T8, 49;

(4) N. Grevesse, A. Noels, A.J. Saural (1996), in *Cosmic abundances*, ASP Conf. Series 99, 117;

* Grevesse et al. (1996) actually suggest 3.55(-4) for the carbon abundance but this value is inconsistent both with interstellar dust modeling (see text) and with comet coma abundances.

abundance. The lower abundance of carbon relative to oxygen as suggested by Grevesse et al. (1996) gives $C : O \approx 0.48$ whereas previous evaluations generally gave $C : O \approx 0.6$. This turns out to be a major difference when one considers the fact that the interstellar dust depletes more carbon than oxygen to the extent that too little carbon is available for the molecules in the gas phase. Concomitantly, as seen in Li & Greenberg (1997), it poses an impossible constraint on the dust given the abundance of gas phase molecules. Consequently, in my judgment, the value of the carbon abundance should be raised so that, as in the past evaluations, the ratio of carbon to oxygen is $C : O \approx 0.6$.

3. Interstellar and precometary dust

The basic model of interstellar dust consists of three populations of particles (Li & Greenberg 1997). The major mass is in tenth micron particles consisting of silicate cores with organic refractory (complex organic molecules) mantles. Additionally there are very small carbonaceous particles/large molecules. In molecular clouds the large particles accrete additional mantles of frozen molecules and in the dense clouds there is also accretion of the very small particle along with the “ices”. This is schematically shown in Fig. 1. The nature of the organic mantle material varies depending on whether the dust is in a low density diffuse cloud or a molecular cloud (Tielens et al. 1996; Greenberg & Li 1997). There are significant variations in the relative proportions of C, N, O and H in the complex organics in different regions. In diffuse clouds the organic mantle is strongly depleted in oxygen and hydrogen, whereas in molecular clouds complex organic molecules are present with more abundant fractions of

Table 2. Stoichiometric distribution of the elements in laboratory organics compared with the comet Halley mass spectra of the organics alone normalized to carbon (Greenberg & Li 1997, Krueger & Kissel 1987, and Krueger private communication).

	Lab Organics			Halley		
	Volatile [†]	Refractory [†]	Total	PICCA(gas)	Dust	Total [‡]
C	1.0	1.0	1.0	1.0	1.0	1.0
O	1.2	0.6	0.9	0.8	0.5	0.6
N	0.05	> 0.01	>0.03	0.04	0.04	0.04
H	1.70	1.3	1.5	1.5	1.0	1.2

[†] Division between volatile and refractory is here taken at a sublimation temperature less than or greater than ~ 350 K respectively.

[‡] Assuming equal amounts of dust (refractory organics) and gas (relatively volatile organics).

oxygen and hydrogen. Furthermore, the ratio of the mass of organic mantles to the silicate core is highly variable. In the unified model for diffuse cloud dust of Li & Greenberg (1997) this ratio is $V_{OR}/V_{sil} = 0.95$, whereas matching the silicate polarization in the Orion B-N object requires $V_{OR}/V_{sil} \approx 2$ (Greenberg & Li 1996). It is of interest to note that the mass spectra of comet Halley dust – as obtained by Kissel & Krueger (1987) and presumably representing the ultimate molecular cloud collapse phase – gave about equal masses of organics and silicates in the dust which implies a volume ratio of about 2. At the other extreme is the region towards the galactic centre which appears to have a very low ratio $V_{OR}/V_{sil} \approx 0.23$ (Tielens et al. 1996). We shall assume that the organic refractory mantles in the final stages of cloud contraction are most closely represented by the properties obtained for Halley dust; i.e. $M_{OR}/M_{sil} = 1$ and with an atomic distribution as given in Table 2 for comet dust organics.

4. Constructing the comet nucleus

4.1. Total mass

If one combines all of the major condensable elements in Table 1, column 4, the total mass (as a mean molecular weight) is $\sum M_i (n_i/n_H) \approx 222.6$. We know that some hydrogen will be present, mostly in combination with oxygen and carbon. Except for an expected large depletion of H by about 650 and an N depletion by about 3 the composition of comet Halley (dust plus gas) is very similar to the solar system abundances (Jessberger & Kissel 1991). In order to account for the full mass of the comet nucleus we have to include some hydrogens. The estimate we make does not strongly influence the end result. We estimate the number of hydrogens as two for each oxygen in H_2O and 0.5 for each carbon in the comet. Since a fraction of the oxygen is in both the organic material and in such volatiles as CO and CO_2 we estimate that only about $\frac{1}{2}$ of the oxygens are in the H_2O so that the total number of hydrogens in the nucleus is approximately $3 \times 2 + 0.5 \times 4 = 8$. The total molecular weight of the comet nucleus material is then

$$M_{C.N.} = \sum M_i (n_i/n_H) + 8 \times M_H = 231. \quad (1)$$

We shall see that an insignificant error is introduced even if we have made an error in the hydrogen number. In reality it will

turn out that the hydrogen number estimate we have made will be consistent with the ultimate material composition.

4.2. Mass of the rockies

It is known that not all the rocky elements are consumed in the silicate cores of the core-mantle particles (Li & Greenberg 1997). However, it is reasonable to expect that all of the rocky elements must be depleted in refractory materials which we generically define as silicates in the comet nucleus composition fraction. We assign four oxygens for the average of the Mg, Si, Fe abundances (based on olivine). This gives a “silicate” mass of

$$M_{sil} = \sum M_r (n_r/n_H) + 4 M_O < (n_r/n_H) > = 59.6; \quad (2)$$

$$f_{sil} = M_{sil}/M_{C.N.} = 59.6/231 = 0.26. \quad (3)$$

Where the subscript r refers to rockies and $<>$ represents mean value. We have accordingly used up all the rockies and depleted the oxygen in the “silicate” by $4 \times (n_r/n_H) = 4 \times 0.35 = 1.4$ so that the remaining abundances are as in Table 3 column (2).

4.3. Mass of the organic refractories (O.R.)

4.3.1. From comet dust mass spectra to comet organics

Instead of letting $M_{OR}/M_{sil} = 1$ based on the dust mass spectrum of comet Halley GIOTTO/VEGA data (Kissel & Krueger 1987) we suggest that $M_{OR}/M_{sil} < 1$. This allows for the fact that some of the rocky elements in the mass spectra appear in combinations other than in silicates: e.g., FeS. Thus for purposes of estimation of the O.R. mass we restrict the silicate core material to that as defined in Li & Greenberg (1997); i.e., to a non-total depletion of the rockies, about 0.87 of the total. We therefore let the fractional mass of the organics to the total comet mass be $f_{OR} = 0.87 \times 0.26 = 0.23$ instead of 0.26.

The depletions of the various elements in the organic mantle component are then obtained by using the comet Halley dust organic mantle reference (mass spectra) abundances as in Table 2: C : O : N : H = 1 : 0.6 : 0.04 : 1.2. It should be noted that the relative abundance for comet Halley dust in Table 2 are

Table 3. Initial and depleted abundances in units $10^{-4}n_H$ after sequentially subtracting the comet nucleus components.

Element	1	2	3	3a	4
	S.S.	-sil	-OR	-OR	-Volatile
C	4.44	4.44	2.2	1.90	1.64
N*	0.61	0.61	0.52	0.51	?
O	7.4	6.0	4.66	4.46	-
Mg	0.38	-	-	-	-
Si	0.36	-	-	-	-
S*	0.16	0.16	0.16	-	?
Fe	0.32	-	-	-	-

* – There is insufficient data to follow the nitrogen and sulfur abundances completely.

for the organics alone so that they are not to be directly compared with those in Jessberger & Kissel (1991) which include the silicates as well. Thus

$$f_{OR} = 0.23$$

$$= (A/231) \times$$

$$4.44 \times (12 + 0.6 \times 16 + 0.04 \times 14 + 1.2) \quad (4)$$

from which $A = 0.50$. The C, O, N abundances, left over after accounting for the organic refractory component, are $(C/H) = (1 - 0.5) \times 4.44 = 2.22$, $(O/H) = 6.0 - (0.5 \times 0.6 \times 4.44) = 4.66$, $(N/H) = 0.61 - (0.5 \times 0.04 \times 4.44) = 0.52$ and are shown in column (3) of Table 3.

4.3.2. From laboratory organics to comet organics

The laboratory organics' relative atomic constituents in Table 2 were based on what are called first generation organics (Briggs et al. 1990). This means that they are a bit too rich in both O and H as can be seen by comparison with the comet Halley data which is probably representative of a mixture of highly photoprocessed diffuse cloud organics with an outer layer of first generation organics created in the final presolar molecular cloud phase (see Fig. 1). Nevertheless it may be instructive to compare the resulting comet abundances which we do by following the same procedure as with the Halley data input. The modified depletion pattern is shown in the Table 3 column 3a. The final consequences on the comet abundances turn out to be small.

4.4. Mass of the ices

4.4.1. From volatiles in the coma back to ices in the nucleus

In contradistinction to the first method used in Greenberg (1982) to derive the comet composition purely as a forward extrapolation from molecular cloud dust, we here work backwards from the comet coma to the nucleus. The molecules in the coma (see Table 4) are much better known now and, indeed, do appear consistent in the general pattern with those observed in molecular cloud dust (see Table 5).

Referring to the summary of observations of coma molecules in Table 4 it is seen that the major fraction of the

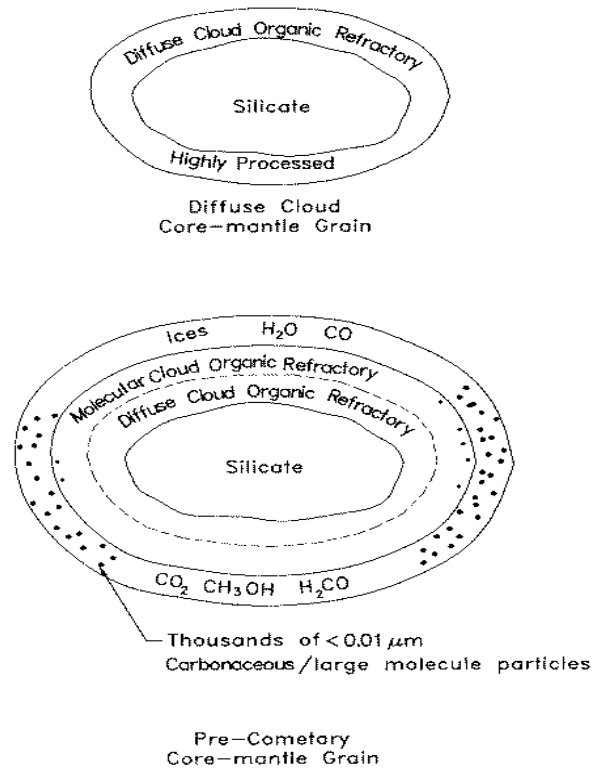


Fig. 1. A schematic description of the morphological and chemical structure of core-mantle interstellar dust grains in diffuse cloud regions and in the latest stage of the collapse of an interstellar cloud. The ices are both accreted and created along with the molecular cloud organics. The very small particle/large molecule components of the interstellar dust accrete along with the ices in the dense cloud.

oxygen and carbon can appear in 6 species. We also note a very substantial spread in abundances for each of them as normalized to H_2O . It will turn out that, because of the constraint imposed by the initial atomic abundances the volatile comet components, particularly H_2O , are limited to a rather narrow range no matter which values we choose. With respect to the CO we should consider that some rather large fraction does not come directly from the volatile nucleus component but is distributed as if coming from heated dust organics (Greenberg & Li 1997). We shall consider a median value for all the volatile components except for CO, for which we take $\frac{1}{2}$ of the median value as being initially volatile. We thus let the volatiles in the coma be as $H_2O : CO : CO_2 : CH_3OH : CH_4 : H_2CO = 100 : 5 : 4 : 3 : 1 : 1$. In this case the volatiles have $C : O = (5 + 4 + 3 + 1) / (100 + 5 + 8 + 3 + 1) = 0.12$ which is within the range of 0.1 – 0.2 generally observed. Clearly a very large fraction of the carbon relative to oxygen is bound up in the organics. Note that if we had assumed that all the coma CO originated in the nucleus we would have obtained $C : O = 0.15$. Let us assume that the volatile coma molecules contain all the remaining available oxygen. This implies that the associated depletion of carbon is 0.12×4.66 which, when subtracted from the available carbon leaves $(C/H) = 1.64$. Since the small car-

Table 4. Molecular abundances in the coma of comets*.

Molecule	C/Hyakutake at 1 AU	Others at 1 AU
H ₂ O	100	100
CO	5-30	2-20
CO ₂	≤ 7	3-6
CH ₄	0.7	≤ 0.5-2
C ₂ H ₂	0.3-0.9	
C ₂ H ₆	0.4	
CH ₃ OH	2	1-7
H ₂ CO	0.2-1	0.05-4
NH ₃	0.5	0.4-0.9
N ₂		0.02
HCN	0.15	0.1-0.2
HNC	0.01	
CH ₃ CN	0.01	
HC ₃ N	≤ 0.02	
H ₂ S	0.6	0.3
OCS	0.3	≤ 0.5
S ₂	0.005	0.02-0.2
SO ₂		≤ 0.001

* – taken from D. Bockélee-Morvan, 1997, in: Molecules in Astrophysics: Probes and Processes (E.F. van Dishoeck, ed.), IAU Symp. 178, Kluwer, 222

bonaceous particles are predominantly carbon one finds for their total mass $M_{\text{carb} + \text{PAH}} = 1.64 \times 12$ and the fraction of the comet nucleus mass in very small carbonaceous/large molecule particles is $f_{\text{carb}} = 0.086$. The fraction of the total available oxygen for H₂O is $100/(100 + 5 + 8 + 3 + 1) = 0.85$ and the associated H₂O mass is

$$M_{\text{H}_2\text{O}} = 0.85 \times 4.66 \times 18 = 71.7 \quad (5)$$

so that the H₂O mass fraction is

$$f_{\text{H}_2\text{O}} = 71.7/231 = 0.31. \quad (6)$$

We may similarly derive the mass fractions of CO, CO₂ and CH₃OH. This completes our inventory of comet nucleus chemical components as summarized in Table 6.

It is important to note that so long as one assumes a comet CO abundance relative to H₂O of 5 – 10% the fractional mass of H₂O in a comet nucleus does not vary by more than 0.02.

4.4.2. From ice mantles in molecular cloud dust to ices in the nucleus

It is often stated that the interstellar dust ice mantles contain molecular species which are a reasonable facsimile of comet coma species. In fact it is suggested that if the dust molecules could be observed up to the time of comet nucleus formation the construction of a nucleus model would be straightforward. The reason for this is that some of the coma molecules are difficult to associate with solar nebula chemistry using partially evaporated interstellar dust; e.g. HNC, CH₄ (Mumma et al. 1993, Irvine et al. 1996). Even though the dust mantle data is limited generally to prestellar molecular clouds or post (massive)

Table 5. Molecules observed in interstellar ice mantles*. Abundances refer to observations of background sources (B), if available. Otherwise, the composition towards high-mass embedded protostellar sources (hmE) is listed.

Molecule	Abundance (%)	Comments
H ₂ O	100	B
CO (apolar)	10-40	B
CO (polar)	1-10	B, hmE
CH ₃ OH	[≤ 4]-10	hmE
CO ₂	[≤ 0.4]-10	hmE, tentative
H ₂ CO	[≤ 1]-10	hmE, tentative
H ₂	≥ 1	hmE
CH ₄	~ 2	hmE, tentative
NH ₃	≤ 10	B, hmE
O ₃	≤ 2	hmE
XCN	?	hmE
OCS/XCS	?	hmE

* – Taken from W.A. Schutte, 1996, in: The Cosmic Dust Connection (J.M. Greenberg, ed.), Kluwer, 1

Table 6. Distribution by mass fraction of the major chemical constituents of a comet nucleus: (a) as derived from comet volatiles, (b) as derived from dust ice mantles.

Materials	Mass Fraction	
	(a)	(b)
Sil.	0.26	0.26
Carb.	0.086	0.092
Organ.Refr.	0.23	0.23
H ₂ O	0.31	0.26
CO	0.024	0.02
CO ₂	0.030	0.03
CH ₃ OH	0.017	0.03
H ₂ CO	0.005	0.02
(other)	0.04	0.05

star formation regions we believe it is instructive to demonstrate the extent to which the comet nucleus molecular pattern is defined as compared with using coma molecules as a starting point. As in the case of coma molecules we note that there is quite a spread in abundances in dust ices. I have chosen high mass embedded protostellar sources rather than molecular clouds as more representative of precometary dust. This is arguable but recall that this is only for comparison purposes. It would be desirable to use data from low mass protostellar sources but this is not available. The relative values for the more abundant molecules which I have abstracted from Table 5 are $\text{H}_2\text{O} : \text{CO} : \text{CH}_3\text{OH} : \text{CO}_2 : \text{H}_2\text{CO} : \text{CH}_4 : \text{NH}_3 : \text{O}_3 = 100 : 5 : 7 : 5 : 5 : 2 : 5 : 1$. The resulting molecular constituent abundances in the comet nucleus are listed in Table 6, column (2). We see, as expected, a small but significant reduction in the total mass fraction of water down to 0.26 but for the rest the changes are not very large. It is evident that a nominal water fraction of about 0.30 is impossible to escape so long as we constrain the comet in terms of the core-mantle dust model and solar system abundances.

5. Discussion

If one accepts the two basic premises that comets are homogeneous aggregates of core-mantle interstellar dust grains and that the comets contain the solar system abundances of the condensable elements the inevitable consequence is that about 30% of the mass of a comet nucleus is H_2O – not much more nor much less is acceptable. While there may possibly be significant variations in the initial comet abundances of the more volatile molecules like CO , CH_3OH , the H_2O abundance is rather strictly constrained. On the other hand, there does not seem to be a clear way of distinguishing whether the observed differences are due to differences in the initial nuclei or are a result of variation in post aggregation evolution such as due to solar heating. The internal consistency of the comet constituent abundances is exemplified by the fact that the derived mass fraction of the small carbonaceous/PAH components is not only as would have been predicted from the interstellar extinction curve but is also consistent with the evidence for the amount of very small (attogram) particles in the coma of comet Halley (Utterback & Kissel 1990).

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