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EXPERIMENTAL EVIDENCE FOR AMORPHOUS CARBON GRAINS IN COMETS

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1. IR SPECTRA OF COMET HALLEY

Ground based observations (Baas et al., 1986; Wickramasinghe and Allen, 1986; Knacke et al., 1987; Danks et al., 1987; Tokunaga et al., 1987) and "in situ" measurements by the IKS telescope on board the VEGA 1 spacecraft (Moroz et al., 1987) have shown the presence of a well pronounced emission feature in the spectrum of comet Halley between 3.3 and 3.7 μm, resolved in different bands (Table 1). This evidence confirms for P/Halley the presence of carbonaceous materials including CH-X bonds, in agreement with measurements by the mass spectrometers PUMA 1/2 and PIA, on board VEGA 1/2 and Giotto, respectively (Kissel et al., 1986; Jessberger et al., 1988).

The band intensity shows temporal variations relative to the continuum: a) on a daily time scale, irregular changes have been observed (Knacke et al., 1987; Wickramasinghe and Allen, 1986; Tokunaga et al., 1987); b) on a monthly time scale, an anticorrelation seems to exist between the band intensity and the continuum level (Baas et al., 1986; Knacke et al., 1987).

A main uncertainty concerns the origin of the bands at about 3.4 μm from either **molecules in gaseous phase** or **solid grains**. However, their broad profile tends to support a solid state origin. Similar absorption features have been observed in the spectrum of various galactic IR sources, as - for example - IRS 7 in Sagittarius A (Butchart et al., 1986) (Table 1). In this last case, carbonaceous grains in dense molecular clouds, close to the Galactic Centre, are considered possible carriers of the bands. Also on the base of the relations between interstellar dust and cometary materials (Greenberg, 1986) a similar attribution for the bands in P/Halley seems possible.

2. HYDROGENATED AMORPHOUS CARBON GRAINS

Hydrogenated amorphous carbon (HAC) grains with mean radius = 40 Å have been produced in laboratory by arc discharge in a controlled Ar atmosphere (p = 1 Torr) between two amorphous carbon electrodes (Bussoletti et al., 1987).

Single atoms or functional groups (H, CH_n, n=1,2,3) may link to chemically unsaturated sites of the crystalline sub-units randomly oriented to form the disordered network (Marchand, 1986). Therefore, weak bands detected in HAC absorption spectra between 3.3 and 3.5 μm are attributed to various C-H bonds (Borghesi et al., 1987). Their wavelength of occurrence and relative intensity suggests a prevalent diamond-like (sp^3) hybridization of the crystallites in HAC grains (Table 1). Dischler et al. (1983) have analyzed the evolution of IR features in α - C:H thin films after thermal annealing, finding a progressive change of the crystalline structure from a dominant diamond-like (sp^3) character, at room temperature, to a prevalent graphite-like (sp^2) type, at 600 °C (Table 1).

HAC grains with variable sp^3/sp^2 content may be produced in space. Since in laboratory experiments this ratio seems to increase with increasing temperature, the $\sim 3.3\ \mu m$ bands from sp^2CH_n are expected to dominate over the $\sim 3.4\ \mu m$ features from sp^3CH_n in HII Regions and Planetary Nebulae, where $T \leq 1000$ K (Sellgren, 1984). The opposite situation occurs in dark clouds and in comets, where the temperature is much lower. The intensity of IR bands measured in laboratory on HAC grains appears much weaker than in space conditions. The large amount of H available in space suggests that various types of **highly hydrogenated amorphous carbon grains (HHAC)** could be among the carriers of both the interstellar and the cometary bands between 3.2 and 3.6 μm.

3. SIMULATION OF COMETARY SPECTRA BY "HHAC"

The best-fit of P/Halley continuum flux recorded on March 30th (Wickramasinghe and Allen) by means of HAC extinction data (Bussoletti et al., 1987, Borghesi et al., 1987) has been obtained for a temperature $T_{g}(HAC) \sim 340$ K, which can be considered as an average temperature of grains emitting in the IR range. The required HAC grain abundance is < 1 % of the total mass rate and ~ 30 % of the rate for grains $< 10^{-5}$ g, well within the limits deduced for carbonaceous grains by PUMA and PIA (Kissel et al., 1986; Jessberger et al., 1988).

To match the 3.4 μm band intensity, HHAC particles have been assumed to have the same optical properties as HAC grains but an H content sufficient to produce a 3.4 μm band stronger than in the HAC case. The Halley spectrum appears well matched if the band intensity is increased by a factor $F = 7$ (Figure 1). To simulate HHAC grains with various sp^3/sp^2 ratios we have scaled the results from Dischler et al. (1983) on the HAC continuum and increased the band intensity by $F = 10$ (Figure 2). HHAC grains with a dominant sp^2 coordination do not reproduce the observations because the 3.28 μm band dominates the 3.4 μm feature, while grains with a sp^3 content ≥ 65 % may account also for the 3.28 μm cometary signature. Therefore, a proper mixture of HHAC grains, with different crystalline structures but a prevalent diamond-like character, is able to give a quite good fit of the IR emission bands detected in P/Halley.

In our picture the IR continuum is attributed to amorphous carbon grains while the 3.4 μm band is due to hydrogenation effects. This scenario may allow to interpret the observed temporal behaviour of the two spectral components: a) the amount of H stuck on grains may suddenly vary in time in the thermodynamically unstationary comet environment, producing daily variations in the 3.4 μm band intensity; b) as the comet removes from the Sun the dust progressively cools down and the relative amount of H trapped onto the grains may rise as well as the 3.4 μm band intensity (monthly variations).

4. SIMULATION OF IRS 7 SPECTRUM BY "HHAC"

The approach used to simulate the cometary bands has been applied to reproduce the absorption bands detected in IRS 7 (Butchart et al., 1986). Also in this case the best-fit has been obtained by HHAC grains, for a band enhancement factor $F = 7$. Again, HHAC grains likely match the 3.4 μm feature, but are not able to reproduce the weaker 3.3 μm band. This goal is achieved when HHAC grains with 33 % of sp^2 content are considered (Figure 3).

5. CONCLUSIONS

Amorphous carbon grains similar to those produced in the laboratory, but with a higher hydrogen content, appear to be good candidates to simulate both the IR continuum emission and the 3.4 μm band measured for P/Halley. The comparison of the cometary features with those detected in laboratory for carbon grains characterized by various sp^2/sp^3 ratios seems to indicate that a prevalent diamond-like (sp^3) structure should be present in cometary particles. This kind of solid particles seem also suitable to explain the daily and monthly variations of the 3.4 μm band intensity, relative to the continuum, and - at the same time - to fulfill the abundance constraints. The same grains appear to be able to reproduce the absorption bands detected in the IR galactic source IRS 7. This result may be considered as a first experimental evidence of a relation existing between interstellar dust and cometary materials.

Baas, F., Geballe, T.R. and Walther D.M.: 1986, Ap. J. (Letters) 311, L97.

Borghesi, A., Bussoletti, E. and Colangeli, L.: 1987, Ap. J. 314, 422.

Bussoletti, E., Colangeli, L., Borghesi, A. and Orofino, V.: 1987, Astr. Ap. Suppl. Ser. 70, 257.

Butchart, I., McFadzean, A.D., Whittet, D.C.B., Geballe, T.R. and Greenberg, J.M.: 1986, Astr. Ap. 154, L5.

Danks, A., Encrenaz, T., Bouchet, P., Le Bertre, T. and Chalabaev, A.: 1987, Astr. Ap. 184, 329.

Dischler, B., Bubenzer, A. and Koidl, P.: 1983, Solid State Comm. 48, 105.

Greenberg, J.M.: 1986, ESA SP-249, 47.

Jessberger, E.K., Christoforidis, A. and Kissel, J.: 1988, Nature 332, 691.

Kissel, J. et al.: 1986, Nature 321, 280.

Knacke, R.F., Brooke, T.Y. and Joyce, R.R.: 1987, Astr. Ap. 187, 625.

Marchand, A.: 1986 in "Polycyclic Aromatic Hydrocarbons and Astrophysics (ed. A. Leger, L. d'Hendecourt, N. Boccara), Reidel Dordrecht, p. 31.

Moroz, V.I. et al.: 1987, Astr. Ap. 187, 513.

Sellgren, K.: 1984, Astrophys. J. 277, 632.

Tokunaga, A.T., Nagata, T. and Smith, R.G.: 1987, Astr. Ap. 187, 519.

Wickramasinghe, D.T. and Allen, D.A.: 1986, Nature 323, 44.

Table 1. Identification of IR bands in space and in laboratory.

Configuration		Laboratory			Observations	
Type	Wavelength (μm)	Band position (μm)				
		HAC	α-C:H		P/Halley	IRS 7
		$T_{ambient}$	50	600 °C		
sp^1CH	3.02		3.03			
sp^2CH (arom.)	3.28			3.28	3.28	3.29
sp^2CH_2 (olef.)a	3.31				3.31	
sp^2CH (olef.)	3.33		3.33			
sp^3CH_3 (asym.)a	3.38	3.39			3.40	3.40
sp^2CH_2 (olef.)s	3.39					
sp^3CH_2 (asym.)a	3.42	3.42	3.42	3.42		
sp^3CH	3.43				3.44	
sp^3CH_3 (sym.)s	3.48	3.48				3.48
sp^3CH_2 (sym.)s	3.51	3.51	3.51		3.51	

Notes: "a" and "s" in column 1 indicate "antisymmeteric" and "symmetric" vibrations; P/Halley and IRS 7 bands: see references in the text.

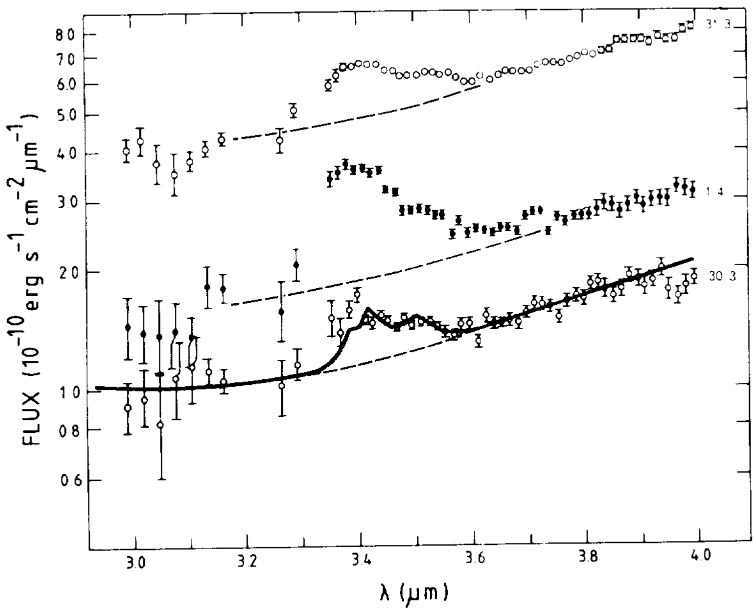

Figure 1. Best fit (solid line) of the 3.4 μm cometary band (Wickramasinghe and Allen, 1986) by means of HHAC extinction data.

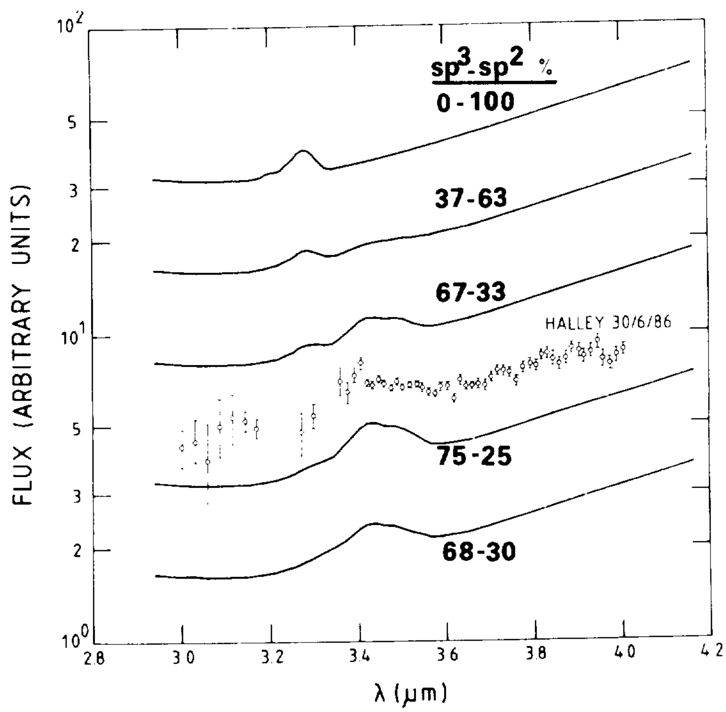

Figure 2. Emission spectra from HHAC grains with various sp^3/sp^2 ratios (Dischler et al., 1983). The Halley spectrum is reported for comparison (Wickramasinghe and Allen, 1986).

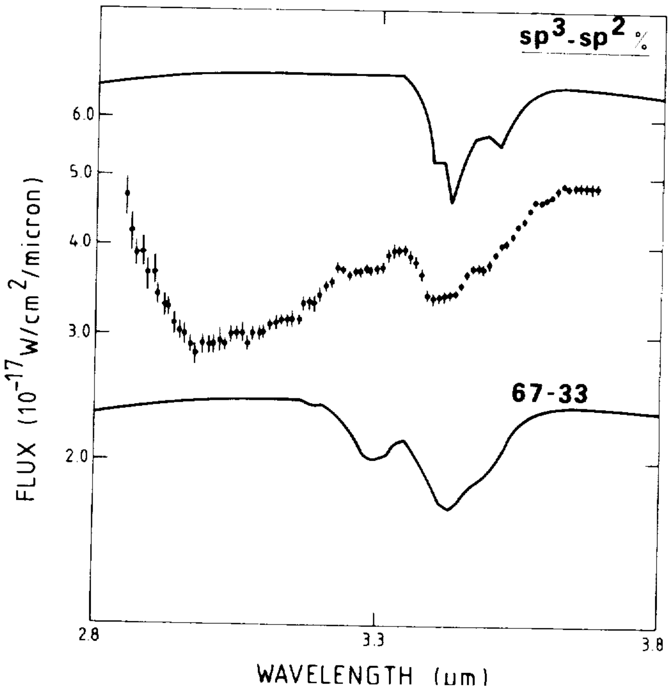

Figure 3. Ordinate displaced best fits (solid lines) of the IRS 7 spectrum (Butchart et al., 1986) by means of the extinction data for HHAC grains with various sp^3/sp^2 ratios.