

THE PAH HYPOTHESIS AND THE EXTINCTION CURVE

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1. THE PAH HYPOTHESIS

The Polycyclic Aromatic Hydrocarbon (PAH) hypothesis states that a *mixture of free* PAH molecules is an ubiquitous and abundant component of the interstellar matter. It has been first formulated by Léger and Puget (1984) on the basis of molecular stability that made PAHs good candidates for the very small grains proposed by Sellgren (1984). Then, they obtained strong, although not final, support from spectroscopy.

2. INTRINSIC DIFFICULTIES TO MAKE A PRECISE SPECTROSCOPIC IDENTIFICATION

They arise because:

- (i) dealing with a mixture of numerous species (see Fig. 1), one cannot expect a sharp spectroscopic fit between the lines of one molecule and the observations such as obtained between the rotational lines of methanol and the corresponding features in radio data. Fortunately, IR spectra have bands that depend almost only on atomic groups and are common to whole families of species (compact PAHs in our case). One cannot expect however a complete agreement unless the exact composition of the mixture is known;

TABLE 1
INTERSTELLAR CONDITIONS COMPARED WITH LABORATORY CONDITIONS

Interstellar	Laboratory
Isolated species	Molecular solids (most data) Isolated (few data- gas phase and rare gas matrix)
Ionized (expected in most present observations)	Neutral
Partially hydrogenated ($\alpha_H \sim 30\%$)	Fully hydrogenated $\alpha_H = 100\%$
Temperatures: 600 - 1000 K	300 K (mostly) 4 - 70 K (matrices) 500 K (gas phase)
Emission	Absorption + calculation Emission: experiment by Cherchneff and Barker (1989)

- (ii) present laboratory analogues of interstellar (IS) PAHs are only approximate. The situation is schematically summarized in Table 1.

3. SPECTROSCOPIC COMPARISON (IR)

From the work of Duley and Williams (1981), Léger and Puget (1984), Allamandola, Tielens and Barker (1985) and Léger, d'Hendecourt and Défourneau (1987, 1988b), it can be concluded that:

- (i) a mixture of compact PAHs can give a reasonably good fit to the whole set of observed features but the 11.3 μm one (see Fig. 11 in Léger *et al.*, 1988b);
- (ii) domination of the 11.3 μm band over the 12 and 13 μm ones can be understood (dehydrogenation);
- (iii) other differences reported in Table 1 do not seem to upset the spectra;
- (iv) emission mechanism is understood.

Several actual predictions of the PAH hypothesis have already been observed:

- (i) mid-IR emission of Cirrus (predicted by Puget *et al.*, 1985 - observed by Boulanger *et al.*, 1985);

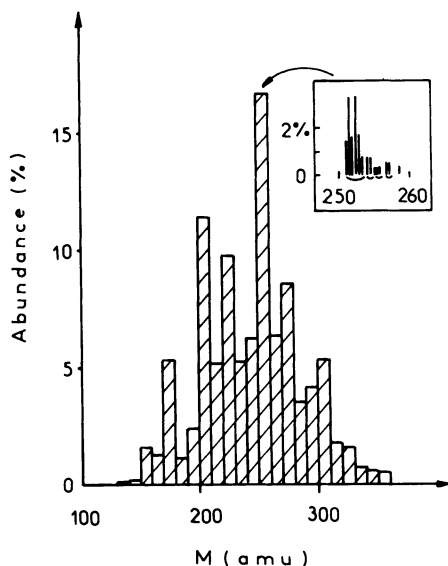


Fig. 1. Mass histogram of the coal pitch extract. Components are gathered in 10 amu bins. The composition of one of them is shown in detail.

- (ii) ubiquity of the $3.3 \mu\text{m}$ feature in the diffuse emission of the Galaxy (predicted by Puget *et al.*, 1985 - observed by the AROME experiment: Giard *et al.*, 1988, 1989);
- (iii) presence of an emission band at $5.3 \mu\text{m}$ (predicted by Léger and d'Hendecourt, 1987 - observed by Allamandola *et al.*, 1989).

Other implications can be searched for in the future:

- (i) presence of a (weak) $1.68 \mu\text{m}$ band, harmonic of the $3.28 \mu\text{m}$ *CH* mode;
- (ii) $12/11.3 \mu\text{m}$ relative importance in cirrus compared to bright reflection nebulae;
- (iii) $158 \mu\text{m}$ *CII*/PAH bands correlation if the IS gas heating is due to the photoelectric effect on PAHs.

4. VISUAL ABSORPTION AND RED FLUORESCENCE

PAH ions have middle to strong absorptions ($f \sim 10^{-1}$) in the visual and are proposed as candidates for the DIB carriers [van der Zwet and Allamandola, 1985; Léger and d'Hendecourt, 1985; Crawford *et al.*, 1985]. Fluorescence processes in PAHs, including Poincaré fluorescence (Léger *et al.*, 1988*a*), are proposed for the red fluorescence observed in reflection nebulae and high latitude HI clouds (Ryter and d'Hendecourt, 1989).

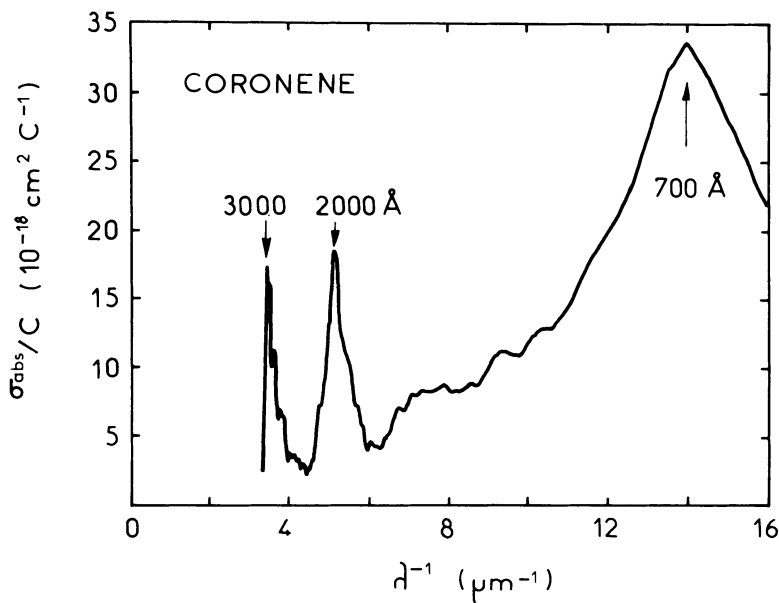


Fig. 2. Absorption cross section of coronene per carbon atom.

5. UV ABSORPTION OF PAH MIXTURES

The PAH hypothesis implies that they absorb in the visual-UV the substantial fraction of the energy that they re-emit in mid-IR. The model by Puget *et al.* (1985) of the IS matter attributes the IRAS 12 μm band diffuse emission to PAHs - in fact, it had predicted it. It represents typically 18% of the total IRAS flux (Boulanger and Pérault, 1988). The 25 μm band emission and about 2/3 of the 60 μm one are also attributed to fluctuating particles (Ryter *et al.*, 1988). The lack of spectroscopical information prevents their precise identification and this situation may last in the future. However, natural candidates are (big) PAHs. They represent 24% of the total.

Thus, PAHs would be responsible for 18% and possibly 42% of the absorption by the IS matter. A question arises: in what part of the extinction curve does it occur? And is there a conflict between the sharp bands of individual PAHs in the UV (Donn, 1968) and their absence in the observations?

We have undertaken UV measurements on coronene and different natural mixtures of PAHs, using the Orsay synchrotron radiation facility (LURE). Mixtures of PAHs are produced by subliming a coal pitch extract whose composition is determined by mass spectroscopy and chromatography (Fig. 1). Due to the high temperature (1400JK) during pitch manufacture, it contains only aromatic species. Over 300 molecules are identified in this PAH mixture and the most abundant ones are only at the level of 3%.

The IR spectrum exhibits sharp 3.3 - 6.2 - 11.3 - 12.0 - 13.5 μm and broad

7.7 μm bands. The extract is vaporized under vacuum in an oven with pinholes for the UV beam and an absolute pressure gauge. A finite sample being vaporized, the vapor composition varies with time as the oven temperature is gradually increased to maintain a constant pressure. This gives us the possibility of studying different mixtures.

The UV cross sections of coronene and PAH mixtures are reported in Fig. 2 and 3. The near UV part of the coronene spectrum agrees with previous measurements in solution (UV Atlas, 1966) but, for the first time, its far-UV absorption is obtained. It exhibits a strong peak at 700 \AA which is also present in benzene and graphite and could be common to all aromatic species.

The absorption curves of PAH mixtures are presently measured only for $\lambda^{-1} < 7.7 \mu\text{m}^{-1}$. They all show:

- little absorption for $\lambda > 4000 \text{\AA}$, $\lambda^{-1} < 2.5 \mu\text{m}^{-1}$
- band gathering in [2500 - 1800 \AA], [4 - 5.6 μm^{-1}]
- depression around 1500 \AA , 6.7 μm^{-1}
- FUV increase for $\lambda < 1500 \text{\AA}$, $\lambda^{-1} > 6.7 \mu\text{m}^{-1}$.

They show a strong similarity with the UV part of the IS extinction curve but for the width of the 2200 \AA bump. Does this latter point only indicate that we have not used a PAH mixture close enough to the interstellar one¹ or is it more fundamental?

6. PAH CONTRIBUTION TO THE EXTINCTION CURVE

Using the above absorption as a guide, let us derive the contribution of PAHs to the IS Absorption Curve from the energy budget. We adopt the analysis of the extinction curve by Greenberg and Chlewicki (1983) that distinguishes: (1) a large grain component and (2) a small "grain" component which is purely absorbing and produces the 2200 \AA bump and the far-UV rise. Using a plausible albedo for large grains and a zero albedo for component (2), we can derive an interstellar *absorption* curve and a global albedo (Fig. 4). The latter agrees well with the values derived by Lillie and Witt (1976) from their study of the diffuse Galactic light. The comparison of Fig. 3 and 4 indicates that PAHs likely contribute to component (2). To what level? The energy budget will give us a strong constraint.

Fig. 5 shows the Interstellar Radiation Field $U_\nu u$ and the power absorbed by the IS matter as:

$$P_\nu = CU_\nu\tau_\nu^{abs} \quad (1)$$

Component (2) is found to absorb about 40% of the total. Now, if PAHs emit and therefore absorb 18%, or 42%, of the total power, *they must be responsible for half, or all, of the component (2) contribution.*

¹For instance, the mass distribution of Fig. 1 is centered at 250 amu whereas the interstellar species are expected to be larger (600 amu), Léger *et al.*, 1988b.

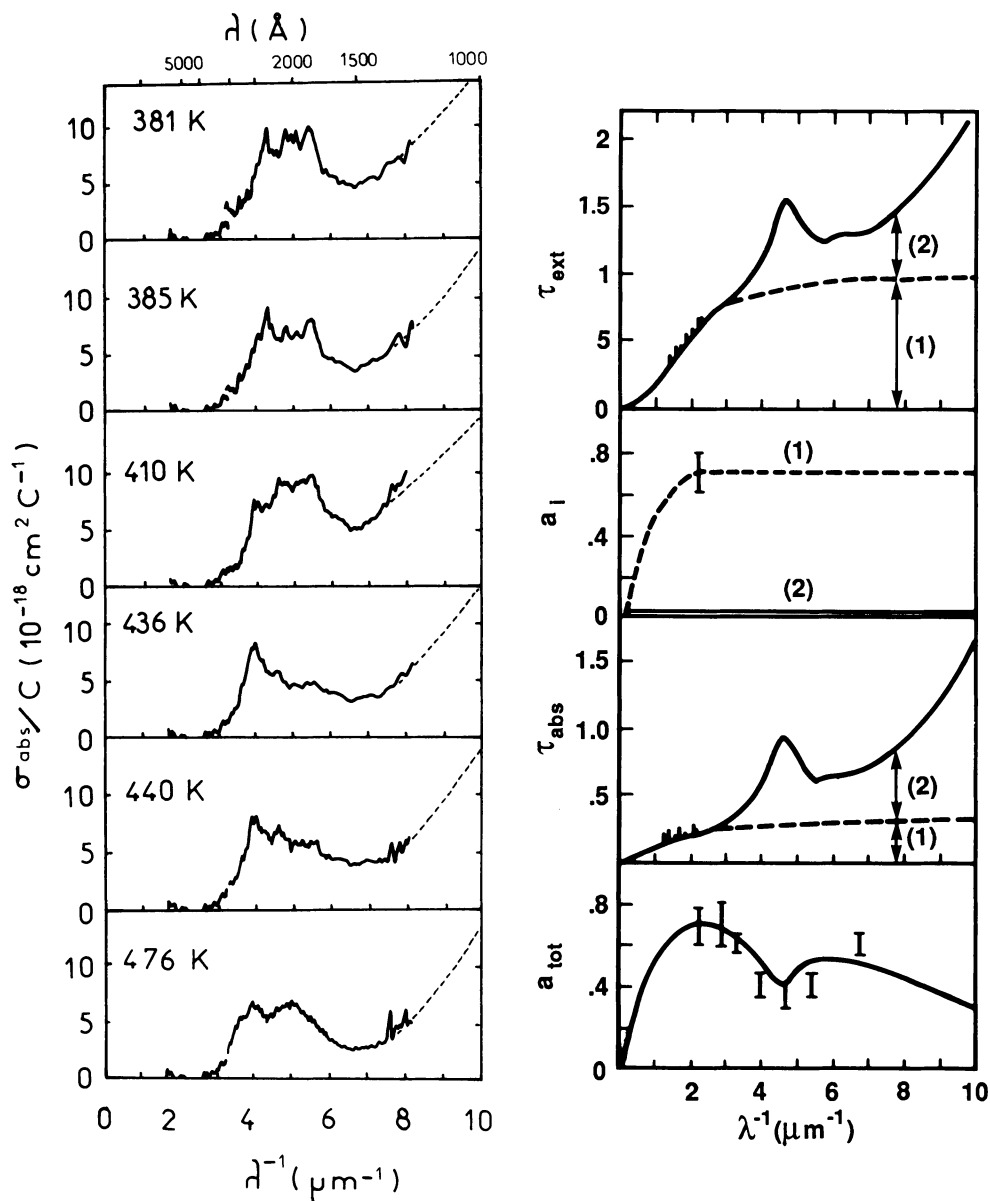


Fig. 3. Left: Absorption cross sections of different PAH mixtures (full line) and coronene (dotted line). The temperature of the oven is reported that determines the mixture as explained in the text. **Fig. 4.** Right: Extinction curve $\tau^{\text{ext}}/(10^{-21}\text{cm}^2\text{H}^{-1})$ analyzed in components (1) (large grains) and (2) with assumed albedos a_1 and a_2 respectively. Resulting absorption curve $\tau^{\text{abs}}/(10^{-21}\text{cm}^2\text{H}^{-1})$ and total albedo. The points with errors bars are values derived by Lillie and Witt (1976) from their observations.

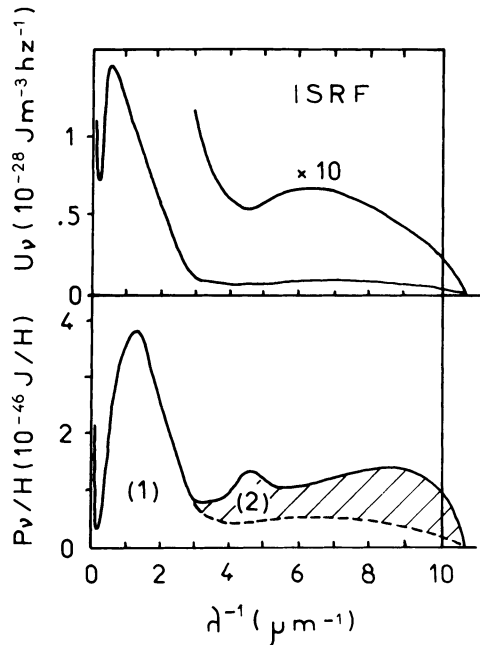


Fig. 5. ISRF spectrum and resulting absorbed spectral power, P_{ν}/H , as a function of λ^{-1} . Contributions of components (1) and (2) are shown separately. The absorbed energy per hydrogen, $\int P_{\nu}/H d\nu$, is found 4.8×10^{-31} W/H, in reasonable agreement with Mathis *et al.*, 1983 (4.2×10^{-31} W/H) and Puget, 1988 (5.7×10^{-31} W/H).

7. IONIZATION CROSS SECTION OF PAHS

The fraction of the absorption cross section which leads to ionization has been measured separately and the implications for the heating of the IS gas by photoelectrons derived. It is reported at this conference by Verstraete *et al.*, 1989.

8. CONCLUSIONS

- The similarity between the UV absorption cross sections of the PAH mixtures measured and the IS absorption curve cannot be considered as a spectroscopic identification because bands are too broad.
- However, if the PAH identification in the IR is accepted, the UV data make a coherent picture as opposed to what the inspection of the spectrum of an individual single PAH spectra may have suggested.
- The energy balance directly implies that PAH molecules are responsible for a significant fraction ($\sim 50\%$), or most, of the 2200 Å bump plus FUV extinction.
- There is a need for performing FUV ($\lambda < 1500$ Å) measurements on PAH mixtures to check whether they show a correlation between the 2200 Å bump and the FUV rise. There is also need for measurement on other (heavier?)

and the FUV rise. There is also need for measurement on other (heavier?) mixtures to check whether the disagreement with the width of the IS 2200Å bump remains.

- The present interpretation of the UV curve predicts a decreasing albedo at wavelengths shorter than 1450 Å.

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