PAHs MOLECULES AND HEATING OF THE INTERSTELLAR GAS

L. Verstraete*,A. Léger*,L. d'Hendecourt*,O. Dutuit**,
D. Défourneau*
*Groupes de Physique des Solides de l'ENS,Université
Paris 7,Tour 23 - 2,place Jussieu - 75251 PARIS Cedex 05
France
**Laboratoire de Physico-Chimie des Rayonnements - Bat.351
- 91405 Orsay - France

Until now it has remained difficult to account for the rather high temperatures (T=80-100 K) observed in many diffuse interstellar clouds (Spitzer and Jenkins,1975).

Various heating mechanisms have been considered: photoionization of minor species (C,Fe,Si) and ionization of H by cosmic rays (Dalgarno and McCray,1972), photoelectric effect on small grains (Jura 1976,Draine 1978). Yet all these processes are either too weak (ionization by cosmic rays, photoionization of trace elements) or efficient under too restricting conditions (photoemission from dust grains) to balance the observed cooling rates (Pottasch et al.,1979). A major heat source is thus still missing in the thermal balance of the diffuse gas.

Recently (Léger and Puget,1984) a new molecular component : the Polycyclic Aromatic Hydrocarbons (PAH),was introduced in the description of the interstellar medium to account for infrared emission features observed in a wide variety of astronomical objects. Those molecules were found to contain about 6% of the cosmic abundance of carbon.

Hence d'Hendecourt and Léger (1987) have reconsidered the problem of the heat input in the diffuse gas and proposed that photoionization of PAHs might be a significant (if not major) heat source. Indeed the photoionization of PAH molecules appears to be very efficient with respect to other processes. This for 2 reasons: first the photoelectron once produced do escape the molecule as opposed to grains in which it has to undergo several scattering processes(Jura,1976), second the recombination cross-section of a PAH is much larger than those for atoms or ions because of the presence of many internal vibrational modes likely to be excited by the recombining electron.Thus the ionization balance results in the presence of a large number of neutral molecules allowing further ionization and heating.

Ionization balance and heating rate per molecule

Following d'Hendecourt and Léger(1987) we write the ionization rate as:

$$R_{ion}= \int_{IP}^{13.6eV} 4\pi F(E)\sigma_{ion}(E)\,dE \tag{1}$$

where F(E) is the mean interstellar radiation field(Draine,1978) , $\sigma_{ion}(E)$ and IP the photoionization cross-section and first ionization potential of the PAH considered
The recombination rate is:

$$R_{rec} = n_e <v.\sigma_{rec}(v)> \qquad (2)$$

where n_e is the electronic density and v, $\sigma_{rec}(v)$ are the speed and recombination cross-section for an electron.The average is to be taken over a Maxwell distribution.
Assuming that the PAH bears a single positive charge and that it is spherical one finds:

$$\sigma_{rec}(v) = Y \sigma_0 (1+ 2eU(a)/mv^2) \qquad (Spitzer,1978) \qquad (3)$$

with $a=0.9\sqrt{Nc}$ Å (Omont,1986) radius of the molecule where Nc is the number of carbon atoms and $\sigma_0 = \pi a^2$ the geometrical cross-section of the PAH , the mean electrostatic potential at r=a is thus defined as U(a) = e/a. Y is the sticking probability for recombination assumed equal to 1 (d'Hendecourt and Léger,1987) and m the electron mass.

After averaging , R_{rec} can be rewritten as:

$$R_{rec}=n_e \sigma_0 (1+ eU(a)/kT) \sqrt{(8kT/\pi m)} \qquad (4)$$

The fractional ionization is then: $\qquad \beta = R_{ion}/(R_{ion}+R_{rec})$
The mean heat input to the gas phase is:

$$Q=(1-\beta)\int_{IP}^{13.6eV} 4\pi dE.F(E).\sigma_{ion}(E)(E-IP).\gamma(E) \quad - \quad n_e\beta <1/2mv^2.v\sigma_{rec}(v)> \qquad (5)$$

where $\gamma(E)$ is the fraction of the energy E-IP that goes in kinetic energy of the photoejected electron.We shall further assume: $<\gamma(E)> = 0.5$, a value inferred from measurements of photoionization of benzene (Terenin and Villessov,1964).
The Maxwell averaged recombined energy is:

$$E_{rec}=n_e.\beta <1/2mv^2.v\sigma_{rec}(v)> = 2kT.\beta.R_{rec}(1 - eU/2kT /(1+eU/kT)) \qquad (6)$$

for the temperatures considered: $\quad eU/kT>>1$, hence:

$$E_{rec} \approx \beta.kT.R_{rec}$$

defining:
$$<E_e> = 1/R_{ion} \int_{IP}^{13.6eV} 4\pi dE.F(E)(E-IP)\gamma(E)\sigma_{ion}(E)$$

as the mean energy of the photoelectron, we can express the heat input per molecule as:

$$Q = \beta.R_{rec}(<E_e>-kT) = <E_e>.\beta.R_{rec}(1 - 2T/3\theta) \tag{7}$$

with : $<Ee> = 3/2k\theta$, defining a mean temperature θ for the ejected electron.

Thus for heating it is necessary that : $T < 3/2\ k\theta$.

Photoionization cross-sections of 2 PAH's:coronene and pyrene

Measurements of the photoionization cross-sections of coronene(C24H12) and pyrene(C16H10) have been carried out using the ACO synchrotron radiation facility of Paris-Sud University.

The experimental process was the following:the species were vaporized in a cylindrical oven where 2 holes were made at both ends to let the light beam through.The photoions where collected on an electrode at -50 V.
The calibration has been performed using absolute cross-sections of ethylene and benzene(Berkowitz,1979) and we dispose now of cross-sections from the IP(~1700Å) up to 600Å for both species.
The cross-sections per carbon atom are presented here below (fig.2) for coronene, pyrene and benzene (as extrapolated by d'Hendecourt and Léger,1987).Note that the cross-sections scaled to the number of C atoms in the PAH are very similar except that of the extrapolated benzene.
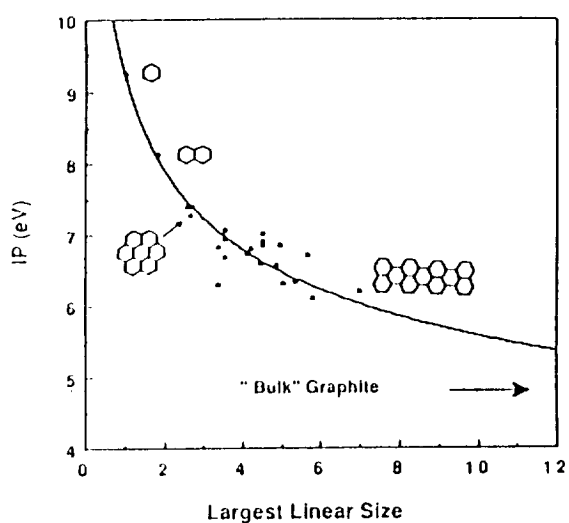

Figure 1 - Ionization potential (IP) of various PAH molecules versus the largest linear size of the molecule in unit of the benzene ring diameter. The reported values are from Eifeld and Schmidt, (1981).
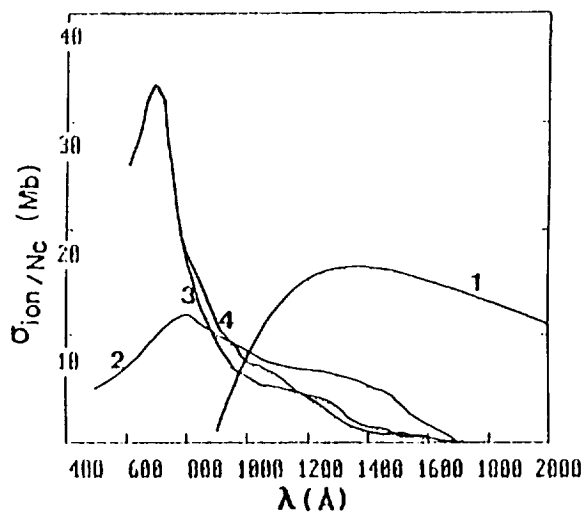
Figure 2: Photoionization cross-sections per C atom in Mb (1 Mb= 10^{-18} cm^{-2}) for benzene (2) as extrapolated by Léger and d'Hendecourt (1987) , pyrene (3) and coronene (4). The mean UV field taken from Draine (1978) is also shown (1).

Heating per molecule and abundance required to balance the cooling of a cold diffuse cloud.

For a cold diffuse cloud with : $T \approx 80K$ $n_e = 3.10^{-2} cm^{-3}$ $n_H = 10 cm^{-3}$ the numerical values found for the ionization fraction, β, the mean temperature of the photoelectron: θ, and the heat input Q/N_C per carbon atom are:

$$\beta = 1.5\% \qquad \theta = 1.39.10^4 \, K \qquad Q/Nc = 1.10^{-21} \, erg.s^{-1}.c^{-1}$$

for both coronene(Nc=24) and pyrene(Nc=16).
Taking a mean cooling rate per H atom from Pottasch et al.:

$$\Lambda/n_H = 1.10^{-25} \, erg.s^{-1}.H^{-1}$$

and assuming thermal equilibrium (cooling rate = heating rate) it is possible to derive what fraction f of the cosmic carbon would have to be carried by PAH's, namely:

$$f = (\Lambda/n_H)/(Q/Nc).(C/H)^{-1}$$

With the above values one finds: $\qquad\qquad\qquad f \approx 25\%$.

This value has to be compared to the abundance deduced from the infrared emission bands.
Léger and d'Hendecourt (Les Houches,1986) found that PAH's would represent 6% of the cosmic carbon in the diffuse interstellar medium and calculated that the mean total number of atoms for a PAH in a reflection nebula should be : $N \sim 50$.
Furthermore Ryter and d'Hendecourt (this meeting) find a minimum size of $N \sim 50$ atoms from an analysis of visible fluorescence in a diffuse HI cloud.
Assuming a hydrogen coverage of 10% for the diffuse medium(Léger and d'Hendecourt,1986) we come to a mean number of Nc ~ 45 carbon atoms.
Our laboratory studies were carried out on smaller species but it is possible to estimate the heat input per carbon for a PAH with Nc =45 from the present data.This can be done assuming that the ionization cross-sections are proportional to Nc (see fig.2 here and Léger and d'Hendecourt,1987) and adopting the empirical evolution of the first IP of a PAH versus its size (fig.1).
Hence the heat input per C atom,and the abundance:

$$Q/Nc = 1.7.10^{-21} \, erg.s^{-1}.c^{-1} \quad and \qquad\qquad f \approx 15\%$$

This latter value is compatible with that inferred from the IR emission features since the IR emission bands should be dominated by the small-size molecules so that the value of 6% should be

considered as a lower limit.
The thermal equilibrium of the warm HI intercloud medium ($T \approx 8.10^3 K$) is not well accounted for (Draine,1978) and it is instructive to estimate the contribution of PAH's to the heat input in such regions.
Assuming $f \approx 15\%$, the same mean energy per photoelectron: 1.8 eV (i.e. $\theta = 1.39.10^4 K$) and taking:

$$T \approx 810^3 K \qquad n_H \approx 0.3 cm^{-3} \qquad n_e/n_H = 0.1$$

the heating rate per H atom turns out to be:

$$\Gamma/n_H = 2.5.10^{-26} \text{ erg.s}^{-1}.H^{-1}$$

This result is comparable to the value of the interstellar cooling function (Dalgarno and McCray,1972) at this temperature:

$$\Lambda/n_H = 3.10^{-26} \text{ erg.s}^{-1} \text{ per H atom.}$$

Conclusion:

Using photoionization cross-sections measured in the laboratory we have shown that in order to balance the observed cooling rates in cold diffuse clouds ($T \approx 80K$) the PAH's would have to contain 15% of the cosmic abundance of carbon.This value does not contradict the former estimation of 6% deduced from the IR emission bands since this latter is to be taken as a lower limit.

Further on we have estimated that the contribution to the heating rate due to PAH's in a warm HI cloud ($T \approx 8.10^3 K$) , assuming the same PAH abundance as for a cold HI cloud , would represent a significant fraction of the value required to keep the medium in thermal balance.

Hence photoionization of PAH's might well be a major heat source for the cold and warm HI media.

It should be noted that the PAH abundance found depends on:

    - the fraction of the incident photon that is converted in kinetic energy of the photoelectron: $\gamma(E)$
    - the recombination cross-section,the mean UV interstellar field
    - the observed cooling rate.
It would be useful to obtain measurements of the cooling function Λ for a variety of regions corresponding to different values of the mean UV energy density and of the near IR fluxes thus allowing a study of the evolution of the heating rate with respect to the size distribution of PAH's.

Finally supplementary laboratory studies are needed for an extension to other PAH species and for the measurement of $\gamma(E)$.

References :

Berkowitz, J.: 1979, Photoabsorption , photoionization and photoelectron spectroscopy , John Wiley and sons

Dalgarno, A., McCray, R.A.: 1972, An.Rev.Astr.& Ap.,**10**,375

Draine, B.T.: 1978, Ap.J. Suppl.,**36**,595

Eifeld, P., Schmidt, W.: 1981, Jal of Electron. Spec. and Related Phenomena,**24**,101

d'Hendecourt, L., Léger, A.: 1987, Astr.Ap.Letters, **180**,L9

Jura, M.: 1976, Ap.J,**204**,12

Léger, A., d'Hendecourt, L.: 1987, in " Polycyclic Aromatic Hydrocarbons and Astrophysics", ed. Léger, d'Hendecourt and Boccara (Reidel: Dordrecht), p.223

Omont, A.: 1986, Astr.Ap.,**164**,159

Pottasch, S.R., Wesselius, P.R., Van Duinen, R.J.: 1979, Astr.Ap. Letters,**74**,L15

Spitzer, L.: 1978, Physical processes in the interstellar medium, John Wiley and sons.

Spitzer, L., Jenkins, F.B.: 1975, An.Rev.Astr.Ap.,**13**,133

Terenin, A., Vilessov, F.: 1964, Adv. in Photochemistry,**2**,385