Identification of the λ2,200A interstellar absorption feature[1,2]

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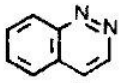
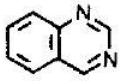
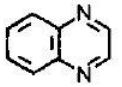
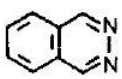
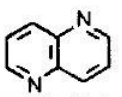
[1]Originally issued as a Cardiff Astrophysics Preprint; published in *Nature*, Vol 270, p.322 on 24 November 1977
[2]First discussion of PAH type molecules in the ISM, as a model for the λ2200A absorption

A broad absorption feature centred at λ2,200A with a half-width of ~300A appears in the spectra of reddened stars[1-3]. This conspicuous feature in the interstellar extinction curve, might hold an important clue to the identity of a major component of interstellar matter, but it has defied identification for over a decade. Here we identify this band as representing the integrated effect of a set of polycyclic compounds, each with the empirical formula $C_8H_6N_2$. Such nitrogenated aromatic structures could form in stellar mass flows of the type which we have also discussed[4]. A significant mass fraction of all interstellar material might exist in this form.

Graphite particles have been considered the most plausible candidate for the λ2,200A absorption feature. Whilst a small particle resonance in graphite can occur close to λ2,200A, the central wavelength of this feature is sensitively dependent on particle shapes. Spherical graphite particles with sizes small compared to the wavelength are necessary to produce agreement with observational data, but a more realistic distribution of shapes would produce a considerably broader absorption feature than is required. It therefore seems that a narrower molecular absorption must be superimposed on an underlying broader extinction hump which could be caused by extinction from graphite grains with a wide spread in their shapes.

Table 1 Properties of various isomers of $C_8H_6N_2$

Compound	Structural formula	λ_m(Å)	ε (molar absorptivity)
Cinnoline		2,250	40,000
Quinazoline		2,220	35,500
Quinoxaline		2,340	23,400
Phthalazine		2,150	56,000
1,5 Naphthyridine		2,060	54,000

We have discussed a possible molecular origin for the λ2,200A band due to $\pi \rightarrow \pi^*$ electronic transitions in a wide class of molecules involving conjugated double bonds[6]. We now limit our search to the nitrogonated heterocyclic aromatic compounds listed in Table l . The first four compounds represent all possible arrangements of two N atoms in a bicyclic structure, with the hetero-atoms confined to one ring only. The fifth compound is an isomer where there is one N atom in each of the two rings.

An average molar adsorptivity function $\langle\varepsilon(\lambda)\rangle$ was computed for these materials from available spectroscopic data[7]. A normalised absorbtivity $A(\lambda)$ given by

$$A(\lambda) = (\langle\varepsilon(\lambda)\rangle - \langle\varepsilon(\lambda_0)\rangle)/ (\langle\varepsilon(\lambda_1)\rangle - \langle\varepsilon(\lambda_0)\rangle) \qquad (1)$$

with $\lambda_0^{-1} = 3.8\ \mu m^{-1}$, $\lambda_1^{-1} = 4.55\ \mu m^{-1}$ is plotted in Fig. 1. Our computed curve for $C_8H_6N_2$ isomers agrees exactly with the interstellar extinction data with respect to the central wavelength, but the 'average' interstellar band is apparently ~ 30% wider. The latter departure could easily be ascribed to an

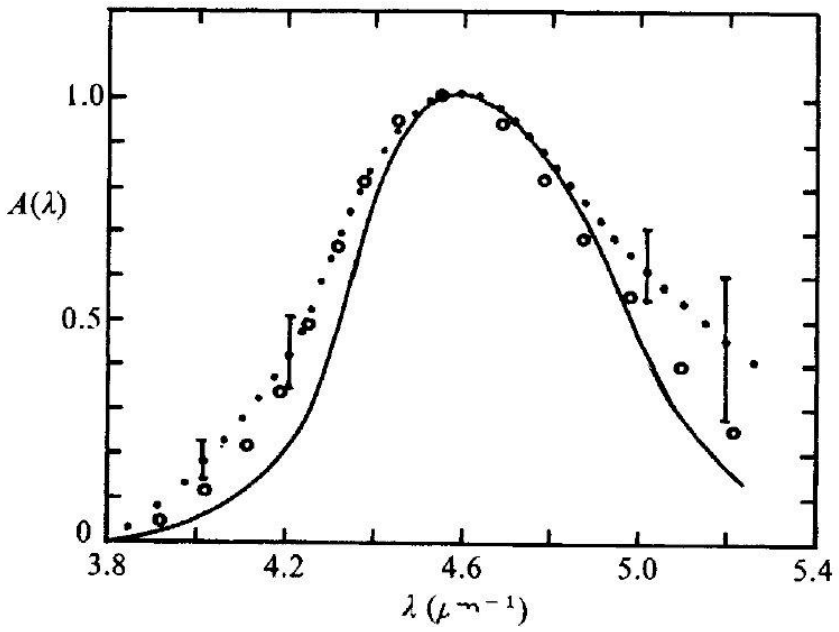


Fig. 1 Normalised average molar adsorptively for $C_8H_6N_2$ isomers (solid curve) compared with interstellar extinction data in the waveband $3.8\ \mu m^{-1} < \lambda^{-1} < 5.4\ \mu m^{-1}$. Normalisation is to 0.0 at $\lambda^{-1} = 3.8\ \mu m^{-1}$, 1.0 at $\lambda_0^{-1} = 4.55\ \mu m^{-1}$. Vertical bars give indication of spread of astronomical data. Dotted curve is the mean extinction curve of Bless and Savage[2] normalised according to equation (1). Open circles give mean extinction ($E(\lambda_V)/E(B- V)$) relative to extinction data for θ-Orionis, and normalised as above.

underlying graphite particulate extinction (scattering+absorption) peak upon which the narrower molecular absorption band is superposed. Since θ-Orionis shows a broad extinction hump centred on λ2,200A rather than the sharper band which is more common, we can reasonably attribute this extinction curve to an underlying graphite component. The mean extinction curve

relative to the extinction data for θ-Orionis (Fig. 1) provides much closer agreement with the molecular absorption data, as we would expect. The mass density of molecules necessary to produce the observed strength of the λ2,200A interstellar band (~1.5 mag kpc^{-1}) is ~ 10^{-27} g cm^{-3} implying that only ~ 10 % of interstellar C and N is in this form.

An identification of polyaromatic compounds of the type listed in Table 1 may have important consequences. Linear molecules such as HCN, HC_3N, HC_5N, HC_7N which have already been observed in interstellar space may result from the break-up of these more complex structures. It would now be worthwhile to search systematically for polyaromatic molecules by radioastronomical techniques.

Sakata et al[8] have reported the detection of an absorption feature at λ2,200A in soluble organic material extracted from the Murchison meteorite. In view of the possible connection of this material with interstellar matter, a chemical analysis of the molecules responsible for the meteoritic λ2,200A band will also be valuable. It is interesting that several nitrogen-bearing heterocyclic compounds, including purines, pyrimidines and pyrroles have recently been identified in carbonaceous chondrites [9-11].

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