

AN INTEGRATED 2.5–12.5 μm EMISSION SPECTRUM OF NATURALLY-OCCURRING AROMATIC MOLECULES*

(Letter to the Editor)

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Abstract. The expected emission features from an ensemble of naturally-occurring aromatic molecules is shown to be in satisfactory agreement with the emission properties of 'PAH molecules' associated with planetary nebulae.

In a recent Letter we pointed out that an ensemble of aromatic molecules derived from natural products would account for both the shape of the 3.3 μm emission feature in NGC 2023 as well as the 2 200 \AA absorption in the interstellar extinction curve (Wickramasinghe *et al.*, 1989). We envisage that such molecules will be contained within fragments of organic grains comprised typically of between 50 and 300 atoms and taking up temperatures in the general range $\sim 1\,200$ to 200 K.

If the constituent molecules of our aromatic ensemble are distributed uniformly over all the grain fragments irrespective of size, the radiation flux arising from the entire ensemble will be given by

$$F_\lambda \sim \bar{\epsilon}_\lambda \left\{ \sum B_\lambda(T) S(T) \right\}, \quad (1)$$

where $\bar{\epsilon}_\lambda$ is the average emissivity and $S(T)$ is the total surface area of fragments with temperature T and $B_\lambda(T)$ is the Planck function. We now proceed to compute the average emissivity of the ensemble listed in Table I over the wavelength range 2.5–12.5 μm .

Each of the laboratory ϵ_λ curves from standard atlases (*Butterworths Index Cards of Spectra*, 1966, 1970, 1972; *Stadler Atlas*, 1978; Scott, 1964) were electronically digitised and scaled so that $\epsilon_\lambda = 1$ at the wavelength of maximum absorption in the 2.5–4 μm waveband. The set of normalised ϵ_λ functions were then averaged with equal weightings to yield a normalised ϵ_λ curve for the entire ensemble.

We next make a simplifying assumption that the distribution of temperatures in Equation (1) averages under the summation sign to give an approximately flat wavelength dependence of the function represented within the curly brackets. In this case $\log F_\lambda$ for an astronomical source would differ from $\log \bar{\epsilon}_\lambda$ by a constant and a direct comparison will be possible. Figure 1 shows the result of such a comparison, with the theoretical curve displaced by an arbitrary amount on the

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TABLE I

Spectra of aromatic naturally occurring organics that were averaged

3-aminoquinoline	N-methyl-2-pyridone
N-methyliminopyridine	3-hydroxypyridine
2-aminoindolenine	Indolenine
Carbinolamine	Corbolineum
Lysergic acid	Indoline
Methylene indoline	8-Indozyl
4-hydroxy-6-methoxy quinoline	9-aminoacridine
8-methylquinoline	Carboxylic acid
Acrylic acid	Methacrylic acid
Mellylcrotonic acid	Sorbic acid
6-methylquinoline	3-picoline
9-ethylcarbazone	Hydroxy lactone
3-hydroxy butenolide	Methoxy lactone
Carbethoxy lactone	Pyridazine
Quinoxaline	4-hydroxy-t-methoxy quinoline
Quinolizone	7-hydroxyquinoline
Dictamnine	Quinolines
2-hydroxyquinoline	2-methoxyquinoline
N-methyl-2-quinoline	1,5-Naphthyridine
2-Oxypurine	Indoxyl
N-acetyldole	N-acylindoline
8 indole	α -pyrone
Alkaloid	Sorbic acid
Lepidine	4-hydroxy-2-methylene lactone
2-methylene lactone	Griseoviridin
7-methylquinoline	Quinaldine
Patulin	Emodin
Anthragallol	Ascorbic acid
Islandicin	Quinazoline
Isoquinoline	6-hydroxy-isoquinoline
N-methyl isoq.	Acridine
Oxindole	Hydroxyacridine
N-methylacridine	Methoxyacridine
Indole	2,3-Dimethylindole
purine	2-aminopurine
2-hydroxypurine	2-methoxypurine
Dimethyl purine	Adenine
Aminopurine	Hydrodypyrine
Methoxypyrimidine	Barbituric acid

TABLE I
(continued)

2-aminopyrimidine	4-aminopyrimidine
Dimethylpyrimidine	Pyrimidines
4-hydroxypyrimidine	5-hydroxypyrimidine
Hydroxy py.	N-methyl py.
N-methyl py.	O-methyl py.
Uracil	Pyridine
Nicotine	3-methylpyridine
2-methoxypyridine	2-hydroxypyridine
3-methoxypyridine	4-methoxypyridine
4-hydroxypyridine	3-aminopyridine
2-aminopyridine	4-aminopyridine
N-methyliminopyridine	2-aminopyridine N-oxide
N-oxidepyridine	Chrysophenol
B-oxybutanolide	Hydroxylactone
Carboxylactone	Butenolide
Acetoxyactone	Cyanodontin
Catenarin	Asperthecin
Acetoxyactone	N-methyl-2-pyridone

TABLE II
Wavelength of principal absorption peaks (μm)

NGC 7027, NGC 2023	3.3	3.4		6.2	7.7	8.6	11.3	
Mixture of aromatics	2.9	3.3	3.4	5.25	6.2	7.7	8.8	11.3

ordinate scale. The observational points are from Sellgren *et al.* (1985). Table II lists the wavelengths of the principal absorption peaks compared with the observed peaks in the astronomical data.

The agreement of the positions of the peaks and the relative strengths of the bands are seen to be generally satisfactory. Departures from the observations seen over the short and long wavelength ends in NGC 7023 are not serious and could easily be rectified by truncating the temperature distribution at a suitable extremal value. Minor modifications of the integrated spectrum, including a suppression of unwanted features (e.g., the 2.9 μm band), might be possible by including the effects of thermal modification of the aromatic ensemble.

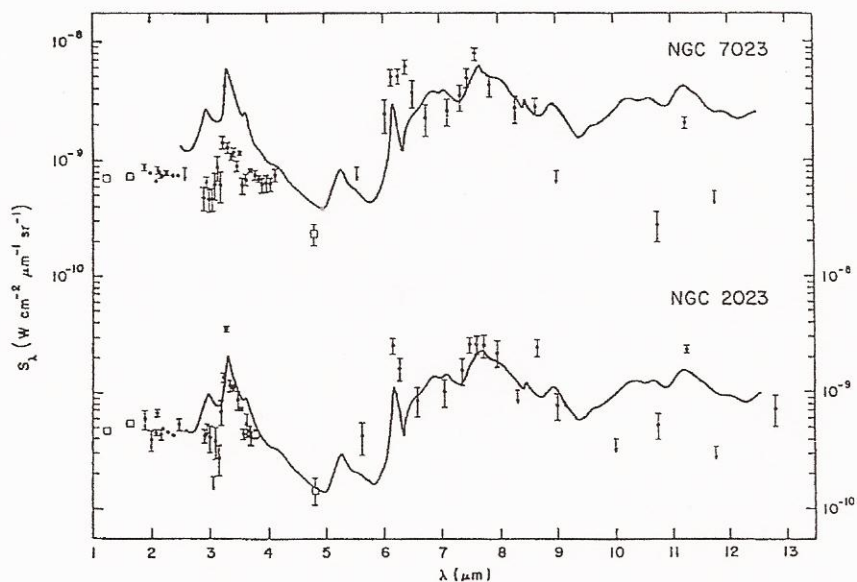


Figure 1. The spectra of NGC 2023 from Sellgren *et al.* (1985) compared to model involving a mixture of 115 aromatic molecules.

References

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