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Ionized Polycyclic Aromatic Hydrocarbons in Space

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The mid-infrared spectrum of a continuously increasing number of stellar objects, planetary and reflection nebulae, H-II regions and extragalactic sources show a distinctive set of broad emission features at 3.3, 3.4, 6.2, 7.7, 8.6, and 11.3 um known collectively as the unidentified infrared emission bands. Although discovered in 1973, identifying the band carrier and elucidating the emission mechanism have been elusive. To date the following models have been suggested to account for the observations: 1) IR fluorescent emission from UV excited molecules on 0.1 um radius grains, 2) IR thermal emission from smaller, 0.01 um grains, and 3) non-equilibrium thermal emission from even smaller 0.001 um grains. All suffer limitations, the first requires a multicomponent mantle composition largely independent of local conditions, the second unusually high values for the infrared oscillator strength and the third relies on the questionable assumption that a 10A sized species can be treated as having bulk thermal properties. Recently, Leger and Puget (1984) proposed that the emission originates in neutral polycyclic aromatic hydrocarbons (PAHs) and used a bulk thermal model to calculate the predicted emission spectrum expected from coronene, which has been "heated" by the absorption of a single photon.

In this poster a model is summarized in which the bands arise, not from grains, or neutral molecules, but from positively charged PAH's on the basis of their low ionization potential and the excellent agreement between the emission bands and laboratory spectra of auto exhaust which contains these types of molecules. These are excited by the absorption of individual U.V. photons, and infrared emission follows as these highly vibrationally excited molecules relax by infrared fluorescence. The emission mechanism must be treated explicitly, taking the statistical nature of the emission process fully into account because each highly vibrationally excited molecule contains a limited number of oscillators with distinct frequencies. This picture, while obviating the need to involve grains or neutral molecules at all, can account for the band intensities, positions and shapes.

The suggested presence of "small" ring containing molecules in space is controversial, and this suggestion has serious ramifications for other spectral regions as well, ranging from the infrared cirrus discovered by IRAS to the classic problem of the diffuse interstellar absorption bands (DIB's) in the visible. Although discovered about 70 years ago, the carrier of the DIB's remains unknown. The interstellar origin of these bands was established in the 1930's when it was shown that the strength of the features did not depend on stellar type, but rather on the amount of extinction, or reddening, toward each star. As the reddening is caused by the intervening gas and dust,

the carrier of the DIB's must be associated with this material. Equally strong cases can be made for a gas phase as well as a solid state origin, but neither explanation is completely adequate. An origin in, or on, the dust implies an asymmetry of the bands which is not observed while a gas phase origin requires large molecules to produce broad bands, yet the presence of large molecules in the harsh interstellar environment seemed impossible. Thus, although an enormous effort has been made observationally, experimentally and theoretically to understand this phenomenon, identifying the carrier of the DIB's has become a classic problem in modern astronomy.

The proposed presence of PAH's in such a variety of objects points to their ubiquitous presence in the interstellar medium. Based on this, we suggest that PAH's are responsible for the DIB's. As pointed out, the interstellar UV field will ionize many of these molecules, changing their electronic structure into that of a radical, which will absorb at discrete wavelengths in the visible. Out of a previously published collection of solid state PAH radical cation spectra we select five on the basis of the unique thermodynamic stability of their carrier and compare them directly to the wavelengths of the DIB's. Although the match seems quite favorable, strongly suggesting that PAH radicals are the long sought after carrier of the DIB's, much laboratory work must be done to test this hypothesis.