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The shape and strength of circumstellar PAH emission bands

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Abstract. We discuss the shape and strength of the emission bands observed in Short Wavelength Spectrometer (SWS) spectra of three carbon-rich evolved stars (Beintema et al. 1996a). The emission bands, due to stretching and bending modes of C-C and C-H bonds in Polycyclic Aromatic Hydrocarbons (PAHs), show large difference in strength and shape, depending on the excitation temperature and size distribution. We find that HR 4049 shows remarkable structure in the major bands (3.3, 6.2, 7.7, 8.6 and 11.3 \mu m) and probably has small, ionized, hydrogen-rich and highly excited PAHs. In contrast, the Planetary Nebulae IRAS21282+5050 and NGC 7027 show a larger abundance of neutral PAHs and plateau emission near 7-8 and 11-12 \mu m, probably due to larger molecules. The population of PAHs in HR 4049 probably has a different evolutionary history than those in the planetary nebulae.

Key words: stars: AGB and post-AGB – stars: mass loss – dust – planetary nebulae – infrared: stars

1. Introduction

The infrared spectra of evolved, carbon-rich stars with temperatures above about 6000 K show emission bands at wavelengths of 3.3, 6.2, 7.7, 8.6 and 11.3 \mu m. These emission bands are attributed to bending and stretching modes of C-H and C-C bonds in complex molecules. The PAH (Polycyclic Aromatic Hydrocarbon) hypothesis has been particularly successful in explaining many of the observed properties of these emission bands, both in circumstellar matter and in the diffuse ISM (for reviews, see e.g. IAU Symposium 135 (1989), Interstellar dust, eds. L. Allamandola & A.G.G.M. Tielens).

Many studies have concentrated on attempts to identify the origin of the observed PAH spectrum with features seen in laboratory measurements of PAH mixtures (e.g. Léger & Puget 1984; Allamandola et al. 1989 (ATB); Jourdain de Muizon et al. 1990; Joblin et al. 1994). These studies are hampered by the unknown composition of interstellar and circumstellar PAHs and differences in excitation conditions between the laboratory and space. It is therefore useful to perform comparative studies of observed PAH spectra in objects with different physical conditions, because this helps to identify the nature of the emission features. Eventually the situation may then be reversed, and observations of PAHs may tell us about the evolution of the object.

Beintema et al. (1996a; hereafter referred to as Paper I) give an overview of the emission features found in the spectra of three well-studied evolved stars, i.e. HR 4049 (a cool post-AGB star), IRAS21282+5050 and NGC 7027 (C-rich planetary nebulae (PNe)). These three objects represent a very wide range in excitation properties: while the effective temperature of HR 4049 is 7500 K, (Lambert et al. 1988; Waelkens et al. 1991a), the temperature of the central star of NGC 7027 is about 160,000 K (Beintema et al. 1996b). We will describe the changes we observe in the spectra of these objects in relation to the excitation conditions. Such studies have been done before using ground-based and airplane data (e.g. Cohen et al. 1986; 1989) and it is clear that what we present here is only a first impression of the potential of the ISO spectra in this area.

2. The observations

The observations were done with the Short Wavelength Spectrometer (SWS; de Graauw et al. 1996) on board ESA's Infrared Space Observatory (ISO; Kessler et al. 1996). The programme stars were selected from the SWS guaranteed time programmes on post-AGB stars and Planetary Nebulae; the spectra...
3. Shape and strength of the emission bands

We focus the discussion on the strongest bands, i.e. the 3 μm region (Fig. 1), the 6 μm region (Fig. 2) and the 7-12 μm region (Fig. 3). These spectral regions contain C-H and C-C stretching and bending modes. We use the strengths of the emission bands as given in Paper I. Note that band strength ratios can be uncertain by up to 50 per cent due to uncertainties in the absolute flux calibration (Schaeidt et al. 1996).

General trends. The emission bands in HR 4049 show significant sub-structure and are narrower than those in the two PNe. This holds for both the C-H and C-C modes. While the bands have weak red wings in HR 4049, these red wings are prominent in the two PNe. The wavelengths of some of the strong bands (6.2, 7.8, 8.6, 9.7, 11.2 μm) in HR 4049 are shifted to longer wavelengths by as much as 0.05-0.18 μm compared to the two PNe. Other bands have quite stable wavelengths, such as 3.29, 6.01, 7.60 and 11.04 μm. There is no evidence for a plateau underlying the "7.7"-8.6 μm or 11.2 μm bands in HR 4049, while such a plateau is prominent in NGC 7027 and IRAS 21282+5050; in the latter object the 11 μm plateau may extend out to ~15 μm (Paper I). The 3.29, 6.2 and 11.26 μm peaks show minor components at 3.248, 6.01 and 11.04 μm. These minor components become less prominent in IRAS21282+5050 and almost disappear in NGC 7027. The "7.7" μm feature is resolved into two separate peaks in all three objects, at 7.60 and 7.72-7.89 μm. In HR 4049 there seems to be a third component at 8.07 μm (Paper I).

Band strength ratios. The 11.2 μm band increases dramatically in relative strength with respect to the 6.2 and 7.7 μm features going from the proto planetary nebulae (PPN) to the
PN phase. Indeed, in NGC 7027, the 11.2 µm band dwarfs the rest of the spectrum. The 7.7/11.2 µm ratio is particularly sensitive to the charge state of the emitting PAHs (DeFrees et al. 1993; Szczepanski & Vala 1993; Hudgins et al. 1994; Langhoff 1996) and very little to the degree of excitation (Schutte et al. 1993). This is well illustrated by a compilation of laboratory-derived spectra of PAH mixtures in different ionization states (Allamandola et al. 1995; Roelfsema et al. 1996). We interpret the observed spectra to imply that the collection of PAHs is almost completely ionized in HR 4049 but partly neutral in NGC 7027. We think that there are several effects that contribute to this general difference in the average degree of ionization. The IR emission from HR 4049 is thought to originate from a circum-binary disk at a distance of only several tens of R_*, (Waelkens et al. 1991b). In contrast, the PAH emission in NGC 7027 stems from the Photo-Dissociation Region (PDR) at 3 x 10^{16} cm from the central star (Graham et al. 1993). As a result the PAH ionizing radiation field (6-8 eV) is more intense in the HR 4049 emitting zone than in NGC 7027. Also, HR 4049 is a late A-type star and has therefore very few CO dissociating and CI ionizing photons (hν > 11 eV), resulting in a low electron abundance (Spaans et al. 1994). In addition, there is reason to assume that the gas/dust ratio in the circumstellar disc of HR 4049 may be low as a result of the accretion of the gaseous component onto the photosphere of HR 4049, resulting in the extremely low metal abundance (Lambert et al. 1988; van Winckel et al. 1992). Thus, the PAH ionization rate may be higher while the recombination rate is lower and hence the overall degree of ionization will be higher in HR 4049 when compared to the PNe.

The band strength variations seem to be limited to the 11.2 µm band, since the 3.3/7.7 µm ratio is similar in all three objects. This is somewhat surprising, since the intrinsic strength of the 3.3 µm feature is predicted to weaken upon ionization (DeFrees et al. 1993; Langhoff 1996), i.e. a weak 3.3 µm feature would be expected in HR 4049. The strength of this feature however is also affected by increasing the fraction of small grains and by multi-photon excitations; both effects tend to decrease the strength of the 3.3 µm C-H stretch (Schutte et al. 1993). Indeed, there is reason to assume that the photon density of the optical/UV radiation field in HR 4049 is high compared to that of the PNe. A much higher excitation is also indicated by the strength of the 3.43 µm 2–1 hot band of the C-H stretching mode in HR 4049 (paper I).

The 6.2 and 11.2 µm bands are distinctly asymmetric in the spectra of NGC 7027 and IRAS21282+5050. These asymmetries are thought to reflect the contribution of hot bands (i.e., 2–1 transition) of these modes which are shifted by anharmonicity to longer wavelengths (Barker et al. 1987). However, given that we concluded that the PAHs in HR 4049, which has fairly symmetric bands, are more highly excited than the PAHs in the PNe, this is likely not the cause of the profile variations. Instead, we attribute these variations to blending with minor features which give the bands in HR 4049 a more symmetric appearance.

**Plateau strength.** The two PNe show strong underlying plateaus in the 7 and 11 µm region which are notably absent in HR 4049. This is however not a general characteristic of PPN versus PN. Some PPN show dominating plateau–like emission features (e.g., AFGL 2688, IRAS22272; Buss et al. 1993). Ground based and air borne studies of such plateaus have shown that they are carried by larger PAHs or PAH clusters containing 300–400 C–atoms (cf., ATB). Thus the spectra indicate a higher proportion of small PAHs in HR 4049 than in the two PNe. This may also explain the enhanced 3.3 µm strength in HR 4049. Perhaps, in the disk environment of HR 4049, shattering by grain–grain collisions is relatively more important (cf., Jones et al. 1994) than in the outflows associated with IRAS21282+5050 and NGC 7027 (or GL 2688 and IRAS22272).

4. Conclusions

The SWS spectrum of HR 4049 does not resemble that of the PNe IRAS21282+5050 and NGC 7027 in detail. The population of PAHs in HR 4049 seems highly excited, ionized and devoid of large molecules. The PAHs in the two PNe show evidence for the presence of large (300–400 C atoms) PAHs, and a significant abundance of neutral PAHs. Apparently, in HR 4049 the proximity of the exciting star results in a high optical/UV photon density which can cause multiple excitations in the PAH molecules. The lack of large PAHs in HR 4049 may be the result of strong processing of the material in the circum-binary disc, either by collisions or by optical/UV photon processing. The disc in HR 4049 is probably Keplerian or at least not expanding, since the velocity of the circum-binary gas is found to be at the systemic velocity (Lambert et al. 1988; Waelkens et al. 1991b). The differences in the PAH spectra of HR 4049 and the PNe therefore probably reflect the very different effects of radiation and grain–grain collisions on a stationary disc (HR 4049) and a detached, expanding cool AGB remnant (PNe). It is possible that in HR 4049 the timescale for processing is longer than that in the PNe, and in fact the HR 4049 PAHs may resemble those more seen in the discs surrounding young Herbig Ae/Be stars (see e.g. Waelkens et al. 1996). Indeed, HR 4049 is the only evolved star in which the 3.52 µm feature, seen in several young objects, is detected (Geballe et al. 1989).

Interestingly, the UV spectrum of HR 4049 does not show evidence for a 2175 Å bump but does show a steep far-UV rise in the extinction (Waters et al. 1989; Buss et al. 1989). The carrier of the 2175 Å bump is believed to be small C-rich grains, and in order to fit the remarkably constant wavelength of the 2175 Å feature along very different lines of sight in the ISM, a restricted size distribution of about 0.02 µm grains is required (Whittet 1992). Apparently this component is missing in HR 4049, but the SWS spectrum suggests that very small particles (PAHs) are abundant. Therefore small PAHs probably are not the carriers of the 2175 Å feature, but likely are contributors to the far-UV rise.

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