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The rich spectrum of circumstellar PAHs

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Abstract. We present observations taken with the Short Wavelength Spectrometer (SWS) on board the Infrared Space Observatory (ISO) of three evolved C-rich stars, the post-AGB star HR 4049 and two planetary nebulae, IRAS21282+5050 and NGC 7027. The spectra are dominated by the well-known infrared emission bands, attributed to Polycyclic Aromatic Hydrocarbons (PAHs). The SWS spectra for the first time allow a complete overview of the richness of the PAH spectrum with high spectral resolution and high S/N. We present an inventory of the spectral features in the 2.4–17 μm wavelength window.

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

1. Introduction

The presence of infrared emission bands at 3.3, 6.2, 7.7, 8.6 and 11.3 μm in the spectra of C-rich evolved objects has been known for over two decades (see e.g. Interstellar Dust, IAU symposium 135 (1989), eds. L.J. Allamandola & A.G.G.M. Tielens). These bands are due to C-C and C-H stretching and bending vibrations in an aromatic hydrocarbon material and various compounds have been proposed, which all have an aromatic microstructure in common (ie., PAHs, QCC, coal; Léger & Puget, 1984; Allamandola et al. 1985; Sakata et al. 1987; Papoular et al. 1989). Analysis of the energetics of the excitation/emission process has now firmly established that the carrier is quite small (≈ 50 C-atoms) and hence is properly referred to as PAH molecules (cf., Allamandola et al. 1989; hereafter referred to as ATB).

In this paper we present ISO-SWS observations of (proto) planetary nebulae ((P)PNe). We have selected three well-studied objects with a large range in excitation conditions, and for which high-quality ground-based spectra already exist, i.e. HR 4049 (e.g. Waters et al. 1989; Geballe et al. 1989; Roche et al. 1991; Buss et al. 1993) IRAS21282+5050 (e.g. de Muizon et al. 1986; Nagata et al. 1988; Witteborn et al. 1989; Jourdain de Muizon et al., 1990; Roche et al. 1991; Justtanont et al. 1996) and NGC 7027 (e.g. Gillett et al. 1973; Russell et al. 1977; Geballe et al. 1985; Nagata et al. 1988; Witteborn et al. 1989; Lowe et al. 1991; Sandford 1991). We present an inventory of the observed emission bands and a comparison with published data. We identify the emission bands in terms of the PAH hypothesis, but we stress that other components may also contribute to the bands. In an accompanying paper (Molster et al. 1996) we discuss shapes and strengths of some of the more prominent bands.

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). Here we concentrate on the emission bands. Data reduction was carried out using version 4.1 of the SWS off-line processing pipeline. Flux calibration is believed to be accurate to about 10 percent at the shortest wavelengths, and 30–50 percent at 30–45 μm (Schaeidt et al. 1996). For a description of the wavelength calibration of SWS we refer to Valentijn et al. (1996). Figure 1 shows the spectra, rebinned to a resolution of 500, and Figure 2 the continuum subtracted spectra. We found that it is difficult to draw the continuum for NGC 7027 between 5 and 14 μm because the spectrum is dominated by emission bands. In Figure 1 two possible continua are drawn and Figure 2 shows the subtracted spectra for both cases. Note the richness in emission bands.
Table 1. Summary of observed bands

<table>
<thead>
<tr>
<th></th>
<th>HR 4049</th>
<th>IRAS21282+5050</th>
<th>NGC 7027</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\lambda_{\text{max}}) ((\mu)m)</td>
<td>(F_{\text{v}}) (Jy)</td>
<td>(\text{FWHM} F_{\text{v}}) ((\mu)m)</td>
<td>(\lambda_{\text{max}}) ((\mu)m)</td>
</tr>
<tr>
<td>3.248</td>
<td>0.33</td>
<td>0.009</td>
<td>0.12</td>
</tr>
<tr>
<td>3.296</td>
<td>5.13</td>
<td>0.045</td>
<td>9.24</td>
</tr>
<tr>
<td>3.342</td>
<td>0.22</td>
<td>0.021</td>
<td>0.21</td>
</tr>
<tr>
<td>3.423</td>
<td>1.17</td>
<td>0.036</td>
<td>1.77</td>
</tr>
<tr>
<td>3.531</td>
<td>2.34</td>
<td>0.019</td>
<td>1.62</td>
</tr>
<tr>
<td>3.757</td>
<td>1.04</td>
<td>0.024</td>
<td>0.72</td>
</tr>
<tr>
<td>6.010</td>
<td>5.50</td>
<td>0.102</td>
<td>2.80</td>
</tr>
<tr>
<td>6.258</td>
<td>14.5</td>
<td>0.165</td>
<td>26.2</td>
</tr>
<tr>
<td>6.318</td>
<td>2.06</td>
<td>0.024</td>
<td>0.36</td>
</tr>
<tr>
<td>7.602</td>
<td>4.89</td>
<td>0.076</td>
<td>11.4</td>
</tr>
<tr>
<td>8.068</td>
<td>2.00</td>
<td>0.059</td>
<td>0.87</td>
</tr>
<tr>
<td>8.593</td>
<td>1.95</td>
<td>0.077</td>
<td>1.14</td>
</tr>
<tr>
<td>8.679</td>
<td>12.5</td>
<td>0.250</td>
<td>12.8</td>
</tr>
<tr>
<td>9.707</td>
<td>5.06</td>
<td>0.112</td>
<td>3.78</td>
</tr>
<tr>
<td>11.04</td>
<td>7.85</td>
<td>0.102</td>
<td>3.36</td>
</tr>
<tr>
<td>11.26</td>
<td>15.9</td>
<td>0.152</td>
<td>9.75</td>
</tr>
<tr>
<td>11.30</td>
<td>2.07</td>
<td>0.027</td>
<td>0.21</td>
</tr>
<tr>
<td>12.75</td>
<td>5.19</td>
<td>0.487</td>
<td>6.90</td>
</tr>
<tr>
<td>12.63</td>
<td>13.2</td>
<td>0.469</td>
<td>23.6</td>
</tr>
<tr>
<td>13.48</td>
<td>3.80</td>
<td>0.105</td>
<td>0.84</td>
</tr>
<tr>
<td>16.99</td>
<td>13.3</td>
<td>1.087</td>
<td>20.1</td>
</tr>
<tr>
<td>18.02</td>
<td>4.40</td>
<td>0.384</td>
<td>2.58</td>
</tr>
<tr>
<td>17.86</td>
<td>16.2</td>
<td>0.396</td>
<td>10.7</td>
</tr>
</tbody>
</table>
This spectral region is dominated by the strong 3.294 μm feature due to the aromatic C-H stretch. Following the suggestion of Jourdain de Muizon et al. (1990), which was strengthened by arguments of Joblin et al. (1996), we attribute the 3.40 μm band to the asymmetric stretch in methyl groups attached to PAHs. The spectrum of methyl coronene also shows very weak bands near 3.35 and 3.48 μm (Joblin 1992). There is no obvious sign of the three strong ethyl coronene bands in this wavelength region. Based upon the detection of the 2-0 overtone of the C-H stretch in IRAS21282+5050 (Geballe et al. 1994), the feature at 3.435 μm is assigned to the 2-1 hot band of the C-H stretch (Barker et al. 1987). In the same vein, the weak feature in IRAS21282+5050 at 3.59 μm may be due to the 3-2 C-H stretch. HR 4049 shows relatively strong features near 3.43 and 3.55 μm, which may well be the C-H hot bands. In that case, the 2-0 should be readily detectable in this source. Possibly, the smallest PAHs, which dominate the emission in these hot bands, survive better in the weaker UV radiation field of this source. The peak position of the aromatic C-H stretch is somewhat sensitive to molecular structure and internal excitation (cf., Joblin et al. 1995). The weak bands at 3.248 and 3.342 μm could thus be due to somewhat larger, less excited and somewhat smaller, more highly excited PAHs, respectively. There are a number of weaker features in these three spectra. These could be due to C-C overtone and combination bands (ATB). Other identifications are also possible. For example, the weak bands at 3.53 and 3.64 in NGC 7027 could be due to the C-H stretch in aldehydic groups attached to PAHs.

The 5–8 μm region: The strong “6.2” and “7.7” μm bands dominate this part of the spectrum and are assigned to aromatic C-C stretching modes (ATB). HR 4049 and to a lesser extent IRAS21282+5050 show a weak band at 6.0 μm. Perhaps, it is connected to the 3.248 μm feature. In any case, we would assign it to a (weak) C-C mode, possibly in a minor population of PAHs. The strong C=O stretching mode of aldehydic groups also absorbs in the 5.75–6.0 μm region but generally peaks at somewhat shorter wavelength (≈ 5.8 μm; Schutte et al. 1990). The “7.7” μm band shows evidence for two independent components at 7.6 and 7.8 μm (cf., Bregman 1989). The 6.9 μm feature is quite evident in NGC 7027 (cf., Cohen et al. 1985). Non-compact PAHs show prominent C-C modes at this wavelength as do small compact PAHs (i.e., pyrene). However, this band can also be due to deformation modes of peripheral CH3 groups. We also recognize that these narrower features are perched upon a broad plateau which extends from about 5.5 to 10 μm, which is known to vary independently (e.g. Bregman et al. 1989). Perhaps, this plateau is due to blended C-C modes in larger PAH clusters (≈ 300–400 C-atoms). Finally, weak features at 5.23 and 5.65 μm are present in the spectrum of NGC 7027. These have been assigned to combination bands of the out-of-plane C-H deformation modes (Allamandola et al. 1989).

The 8–11 μm region: Bands in this region are due to C-H in-plane deformation modes. The well known 8.6 μm band dominates this spectral region. However, all three sources show evidence for weaker features, whose peak position varies between 9.5 and 10.5 μm depending on the H substitution pattern.
(Bellamy 1970). The observed pattern is consistent with the presence of isolated H's, as inferred from the out-of-plane C-H deformation mode. However, at this point, confusion with stretching vibrations of peripheral C-C and C=O groups cannot be excluded.

The 11–15 μm region: This is the region of the C-H out-of-plane deformation modes, which in interstellar spectra is dominated by the 11.3 μm band (Cohen et al. 1985). The 11.0 μm band may well correlate with the 6.0 and 3.248 μm bands. Bands in this region are very sensitive to the H-substitution pattern. Bands between 11 and 11.6 μm are generally assigned to peripheral H's isolated on the aromatic ring. The 12.7 μm feature is consistent with three adjacent H's (ATB), while the weak 12.1 μm band in IRAS21282+5050 can be assigned to duo H's. These assignments are somewhat under debate since these peak positions seem to be sensitive to ionization (Langhoff 1996) and this effect has not been sorted out completely, yet. The underlying broad plateau in NGC 7027 may represent a blend of various weak out-of-plane deformation modes, possibly connected to the larger PAH clusters. Finally, we note that this emission plateau extends to about 16 μm in IRAS21282+5050 (Justtanont et al. 1996) and that may be difficult to explain with out-of-plane deformation modes.

The long wavelength modes: Presently our data possibly reveal only one band, near 17 μm. This spectral 'poorness' may partly reflect the difficulty to detect (weak) emission features against the "dust" continuum which rapidly increases in strength with wavelength. Also, PAH modes in this wavelength region are intrinsically weak (ATB). Long wavelength bands are due to skeletal vibration and hence, in general, very specific for a particular PAH structure. As a corollary, this implies that, unlike the mid-IR spectral regions, bands from a collection of PAHs do not line up well, further hampering their detection. The 17 μm feature, if real, may well be the in-plane ring deformation mode. The out-of-plane ring deformation mode occurs at lower frequencies. The 21 μm feature observed in some sources may well be related to such vibration, which one might call the drumhead mode, where adjacent rings bend out-of-plane.

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