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SPECTROSCOPY OF THE 3 MICRON EMISSION FEATURES

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ABSTRACT

Spectroscopic observations at a resolving power of ~400 between 3.1 and 3.6 μm are presented of the planetary nebulae NGC 7027, BD +30°3639, and IC 418; the H II region S106; and the red rectangle HD 44179. The well-known emission features at 3.3 and 3.4 μm are resolved. The 3.4 μm feature is found to consist of two components: a sharp feature at 3.40 μm and a broad plateau centered approximately at 3.45 μm. The relative strengths of the 3.3, 3.40, and 3.45 μm features vary from source to source. No evidence for source-to-source variation in the shape of the 3.3 μm feature is found. The new data are discussed in the context of the recent attempts to identify the features.

Subject headings: infrared: sources — interstellar: grains — nebulae: H II regions — nebulae: planetary

I. INTRODUCTION

Infrared spectroscopy of circumstellar and interstellar dust has been an active field of study for more than a decade (see reviews by Aitken 1981 and Willner 1983). At least 15 emission features and a similar number of absorption features have been attributed to dust. Although the absorption spectrum of interstellar dust is moderately well understood, only three emission features, due to silicates and silicon carbide, have well-accepted identifications. Six unidentified emission features, at 3.3, 3.4, 6.2., 7.7, 8.6, and 11.3 μm, are often considered to form a family. These features are almost always found together and appear to be associated with dust near molecular cloud–H II region boundaries.

In this paper we present high-spectral-resolution observations of the 3.3 and 3.4 μm features in the three planetary nebulae NGC 7027, IC 418, and BD +30°3639; the H II region, S106; and HD 44179, the "red rectangle." HD 44179 may be an evolved star rapidly losing mass (Russell, Soifer, and Willner 1978). These data clearly resolve the above two features and point out the existence of a third feature centered near 3.45 μm. Previously, spectra at a resolving power of ~70 were presented for four of these objects by Russell, Soifer, and Merrill (1977). A grating-resolution spectrum of NGC 7027 was presented by Grasdalen and Joyce (1976), and high-resolution FTS spectra of NGC 7027 and HD 44179 were published by Tokunaga and Young (1980); however, the signal-to-noise ratios of those spectra were too low to show the emission profiles of these features clearly.

II. OBSERVATIONS AND RESULTS

Several sets of observations are reported here. Spectra of NGC 7027 and BD +30°3639 were measured with a cooled grating spectrometer with an InSb detector (Persson, Geballe, and Baas 1982) on the Palomar Observatory 5 m telescope in 1983 August. These sources were observed over the wavelength range 3.1–3.6 μm (2780–3210 cm^{-1}) with a spectral resolution of $\Delta\lambda = 0.078$ μm corresponding to a resolving power $R \approx 430$. The aperture diameter was 4″. A position in the H II region, S106, 20″ south of the bright infrared object IRS 3 (Pipher *et al.* 1976) was observed in 1983 July with the United Kingdom Infrared 3.75 m telescope (UKIRT) at Mauna Kea Observatory. A seven-channel (InSb detector) cooled-grating spectrometer (Wade 1983) was used at a resolving power of 450, with a 5″ diameter aperture. This instrument was also used at UKIRT to observe IC 418 and HD 44179 on two nights in 1984 February and BD +30°3639 on one night in 1984 June. The UKIRT observations all cover the range 3.2–3.6 μm (2780–3130 cm^{-1}). In all sets of observations, standard stars were measured close in air mass to the objects in order to remove atmospheric absorption features.

The measured spectra are shown in Figure 1. The BD +30°3639 spectrum is the one obtained at UKIRT; it is consistent with the one obtained at Palomar. All spectra omit a small interval near 3.32 μm (3015 cm^{-1}) where there is strong telluric methane absorption. The UKIRT data have been Hanning (triangle) smoothed, lowering the resolution of those spectra to ~0.095 μm. Estimated continua for NGC 7027, IC 418, BD +30°3639, and HD 44179 are shown as straight lines which match the observed short wavelength points and whose slopes are taken from the low-resolution spectra of Russell, Soifer, and Merrill (1977).

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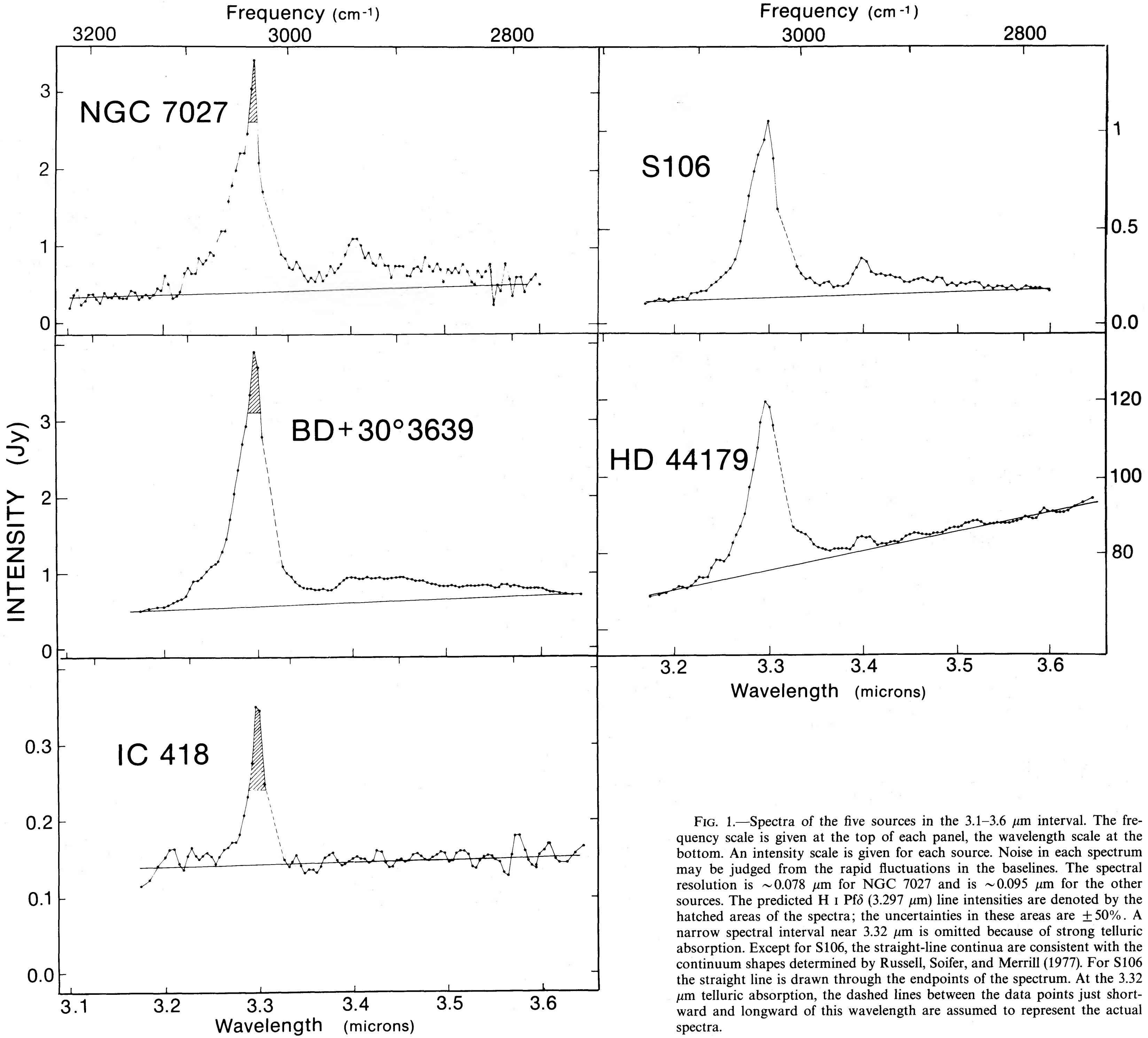

FIG. 1.—Spectra of the five sources in the 3.1–3.6 μm interval. The frequency scale is given at the top of each panel, the wavelength scale at the bottom. An intensity scale is given for each source. Noise in each spectrum may be judged from the rapid fluctuations in the baselines. The spectral resolution is $\sim$0.078 μm for NGC 7027 and is $\sim$0.095 μm for the other sources. The predicted H I Pfδ (3.297 μm) line intensities are denoted by the hatched areas of the spectra; the uncertainties in these areas are $\pm$50%. A narrow spectral interval near 3.32 μm is omitted because of strong telluric absorption. Except for S106, the straight-line continua are consistent with the continuum shapes determined by Russell, Soifer, and Merrill (1977). For S106 the straight line is drawn through the endpoints of the spectrum. At the 3.32 μm telluric absorption, the dashed lines between the data points just shortward and longward of this wavelength are assumed to represent the actual spectra.

a) Resolved Emission Features

Three resolved emission features can be seen in the spectra of these five objects: two rather narrow features which peak near 3.30 and 3.40 μm and a broad plateau extending from $\sim$3.35 μm to $\sim$3.60 μm. The latter two both contribute to what has been referred to in earlier papers as the 3.4 μm feature. Several parameters of the observed features are given in Table 1. Hereafter, we refer to the first two features as the 3.3 and 3.4 μm features, and to the last as the 3.45 μm feature or plateau. The reality of the plateau in NGC 7027 might be questioned, but an independently obtained spectrum of NGC 7027 (Geballe 1984) supports its existence, and it also appears in the spectrum of Merrill, Soifer, and Russell (1975). In addition, the plateau is clearly present in both BD +30°3639 and S106.

The precise peaks, strengths, and shapes of the emission features and their source-to-source variations are not easily determined. Difficulties are created by the presence of the H I Pfδ line near the peak of the 3.3 μm feature in all sources but HD 44179, strong telluric absorption near 3.32 μm, and overlap of the emission features themselves. The contribution of Pfδ at 3.297 μm can be estimated for NGC 7027, BD +30°3639, and IC 418 from their total Brγ line and continuum fluxes (Merrill, Soifer, and Russell 1975; Beckwith, Persson, and Gatley 1978; Willner *et al.* 1979) by scaling the total Brγ line fluxes both by the Case B recombination line intensity ratio, Pfδ/Brγ = 0.24, and by the fractions of the total continuum flux densities observed in the present small apertures. The predicted Pfδ line strengths are given in Table 1 and indicated in Figure 1 by the hatched areas of the spectra near 3.297 μm. The sizes of the hatched areas are uncertain by perhaps ±50% because the Pfδ line and the strong telluric absorption lines in its vicinity were not spectrally resolved.

For the purposes of calculating intensities and equivalent widths, the local minimum at 3.35 μm, which occurs in all the spectra of Figure 1 except that of IC 418, has been defined to be the boundary between the 3.3 μm feature and the 3.45 μm plateau feature. In addition, based on the available spectra of the prominent 3.4 μm emission feature in NGC 7027 (Geballe 1984; this paper), we define this feature to consist of that emission between 3.38 and 3.43 μm in excess of a straight line drawn between the data points at those wavelengths. The underlying continua, on which all equivalent-width determinations are based, are assumed to be the straight lines in Figure 1 which connect the long- and short-wavelength regions of each spectrum. We note the arbitrariness of some of the above definitions. for example the equivalent widths of the 3.3 μm features exclude the contributions of Pfδ but include contributions from the 3.45 μm plateau features if, in fact, the wings of these extend shortward of 3.35 μm.

We now briefly describe each of the three emission features. The 3.3 μm feature has a full width at half maximum (FWHM) of approximately 0.040 μm (37 cm^{-1}). In HD 44179 the peak of the feature occurs at 3.298 ± 0.003 μm (3032 ± 3 cm^{-1}), which is coincident with the Pfδ rest frequency. Removal of the Pfδ contribution from the NGC 7027 and BD +30°3639 spectra suggests that the peak is coincident with Pfδ in those sources as well, but this requires confirmation by higher resolution spectroscopy. Emission drops off more rapidly at wavelengths longward of the peak than shortward in all sources. Thus the emission-weighted mean wavelength of the feature lies shortward of the peak; it is presumably for this reason that occasionally the feature has been reported as occurring at 3.28 μm. The present spectra contain no evidence for source-to-source variation in the shape of the 3.3 μm feature. The faintness of the 3.3 μm emission feature in IC 418 (after correction for Pfδ), and the lack of recombination-line information about the S106 position, lead to uncertainties in the corrected spectra

TABLE 1

3 μm DUST EMISSION FEATURES

Parameter	NGC 7027	BD +30°3639	IC 418	S106	HD 44179
Beam diameter	4″	5″	5″	5″	5″
3.3 μm:					
$\nu_{\rm peak}$ (cm^{-1})	3034 ± 5	3034 ± 7	3034 ± 10	3034 ± 10	3033 ± 3
W_ν (cm^{-1})^{a}	270 ± 30	230 ± 25	21 ± 4	360 ± 40	26 ± 3
$F_{\rm obs}$ (10^{-18} W cm^{-2})^{a}	3.3 ± 0.4	3.9 ± 1.0	0.09 ± 0.02	1.2 ± 0.2	58 ± 6
3.4 μm:					
$\nu_{\rm peak}$ (cm^{-1})	2938 ± 5	2945 ± 7	...	2941 ± 5	2941 ± 7
W_ν (cm^{-1})	16 ± 4	4.5 ± 2.0	<5	18 ± 4	0.8 ± 0.3
$F_{\rm obs}$ (10^{-18} W cm^{-2})	0.21 ± 0.04	0.08 ± 0.03	<0.02	0.08 ± 0.02	1.9 ± 0.7
3.45 μm:					
$\nu_{\rm peak}$ (cm^{-1})	2900 ± 50	2900 ± 50	...	2900 ± 50	...
W_ν (cm^{-1})	85 ± 25	60 ± 20	<20	53 ± 20	2.5 ± 2.5
$F_{\rm obs}$ (10^{-18} W cm^{-2})	1.2 ± 0.4	1.2 ± 0.4	<0.08	0.26 ± 0.10	6 ± 6
Pfδ (3.297 μm):					
$F_{\rm pred.}$(10^{-18} W cm^{-2})^{b}	0.10	0.13	0.05	...	0
Scaling factor^{c}	8	1.1	7	...	1.2

[a] After subtracting Pfδ predicted, except for S106.

[b] Pfδ line strength predicted on the assumptions that I(Pfδ)/I(Brγ) = 0.24 and that the fraction of the total line flux in the aperture equals that of the continuum measured.

[c] The factor by which the 3 μm continuum flux densities in Russell, Soifer, and Merrill (1977) exceed those measured here.

of these objects but not to a contradiction of the above conclusion.

The weaker 3.4 μm feature, which is most prominent in NGC 7027 and S106, peaks at 3.40 μm (2940 ± 3 cm^{-1}) and has a FWHM of approximately 0.023 μm (20 cm^{-1}). It has a rather sharp edge at 3.38 μm and may degrade more slowly to long wavelengths (see also Geballe 1984). The plateau feature is difficult to characterize, due to its faintness. Its intensity appears to vary smoothly, with a peak near 3.45 μm (2900 cm^{-1}). However, its short-wavelength limit cannot be determined because on that side the plateau merges with the much brighter 3.3 μm feature. The long-wavelength limit of the plateau also is not well determined, although emission beyond 3.60 μm is surely weak, if present at all.

Especially noteworthy in these spectra are (1) the existence of the narrow peak at 3.40 μm and the 3.45 μm plateau, whose separate identities have been established only recently in one object, NGC 7027 (Geballe 1984); and (2) the source-to-source variation in the strengths of the 3.4 μm and 3.45 μm features relative to the 3.3 μm feature, which has not been demonstrated previously. The 3.3 μm feature is present in all five objects, although in IC 418 almost half the excess intensity near this wavelength is due to Pfδ (see below). The 3.4 μm feature is relatively prominent both in NGC 7027 and in S106. However, in BD +30°3639 the intensity of the 3.4 μm feature relative to 3.3 μm is much less than in those two sources. Indeed it is only the sharp short-wavelength edge at 3.38 μm which gives away its presence in BD +30°3639. Note that in the low-resolution spectra of Russell, Soifer, and Merrill (1977) NGC 7027 and BD +30°3639 appear very similar near 3.4 μm; it is the higher spectral resolution of the present measurements which reveals their difference. A weak 3.4 μm feature (relative to 3.3 μm) was also detected in HD 44179. In IC 418 no 3.4 μm feature or 3.45 μm plateau was detected, but the limits for these features relative to the 3.3 μm feature after accounting for Pfδ is not significant in this object. Both the present spectrum of HD 44179 and the spectrum of Russell, Soifer, and Willner (1978) imply that the 3.45 μm plateau feature is weak or absent there.

We find no evidence in the three planetary nebulae and in S106 for the 3.43 and 3.53 μm emission features found in HD 97048 by Blades and Whittet (1980) and identified as solid H_2CO by Baas *et al.* (1983). However, the 3.53 μm feature may be present weakly in the spectrum of HD 44179. Because the spectral type of HD 44179 is similar to that of HD 97048, a detection of the 3.53 μm feature would not be surprising. Additional measurements are necessary for confirmation.

b) *Line Emission*

As noted previously, H I Pfδ at 3.297 μm is prominent in the spectra of all sources except HD 44179. Strong telluric absorption apparently prevented Tokunaga and Young (1980) from identifying this line in NGC 7027, and the line could not have been resolved from the 3.3 μm feature in the spectra of Russell, Soifer, and Merrill (1977). In all the observed sources except IC 418, the Pfδ line intensity is very small compared to that of the 3.3 μm feature. The sharpness of the 3.3 μm feature in IC 418 indicates that the line contribution there is substantial. Using the scaling procedure described previously, we conclude that the Pfδ line is responsible for nearly half of 3.3 μm emission which we observed in IC 418. This demonstrates that without some knowledge of the H I recombination-line spectrum, caution must be exercised before attributing the bulk of the 3.3 μm emission observed at low spectral resolution to the 3.3 μm dust feature.

High-order H I Humphreys lines (n–6), which fall across the spectrum from 3.6 μm to the series limit at 3.28 μm, are expected to have only a small effect on the spectra. Several of these lines can be seen in the spectrum of NGC 7027 of Geballe (1984). In the present NGC 7027 spectrum, the Hu 20 line at 3.607 μm should appear as a bump only 0.024 Jy above the continuum at the present spectral resolution, and the integrated Hu line flux from Hu 20 to the series limit should be ~10 times this amount, assuming optically thin lines. Between 3.3 and 3.5 μm, where the Humphreys-series lines are unresolved, they would be expected to produce a relatively flat continuum, as the increasing density of lines compensates for the decreasing A-coefficients for increasing upper state quantum number. Thus, unless the b_{nl} values vary markedly for $n > 20$, Humphreys lines should neither contribute a significant fraction of the 3.3–3.6 μm flux observed nor seriously influence the shape of the 3.45 μm plateau feature. An independent observational argument that the latter is true can be made for NGC 7027 and BD +30°3639. In the present apertures, these two sources have free-free flux densities which exceed that of IC 418 by factors of approximately 5 and 3 respectively (radio fluxes from Walmsley, Churchwell, and Terzian 1981), but their 3.45 μm features are at least 15 times that of IC 418 (Table 1).

Vibration-rotation line emission from H_2 was discovered in NGC 7027 by Treffers *et al.* (1976). The strongest H_2 line in the 3.1–3.6 μm region is likely to be the 1–0 O(5) transition at 3.235 μm (3091 cm^{-1}). This line was observed in NGC 7027 by Geballe (1984), although it is not apparent in the present spectrum. The line appears to be marginally present in BD +30°3639. In neither of these objects are the H_2 lines intense enough to create difficulties in analyzing the broad emission features.

III. DISCUSSION

In addition to delineating the spectral characteristics of the 3.3, 3.4, and 3.45 μm emission features, the most notable results of these observations are the differences between the spectra of NGC 7027 and S106, the spectrum of BD +30°3639, and the spectrum of HD 44179. Previous low-resolution spectra have shown little variation in the relative strengths of the 3.3 and 3.4 μm features among different ionized regions, including NGC 7027 and BD +30°3639. An exception was IC 418, which showed only the 3.3 μm feature. However, the upper limit to the intensity ratio of the 3.4 μm feature and the 3.3 μm feature (excluding Pfδ) in IC 418 is not stringent. Therefore, we exclude IC 418 from the remainder of the discussion. To summarize the relevant results, all three features are prominent in NGC 7027 and S106, only the 3.3 μm feature and 3.45 μm plateau are prominent in BD +30°3639, and only the 3.3 μm feature is prominent in HD 44179.

Upon comparing the various spectra obtained here, we conclude that the 3.4 μm feature is at best only weakly coupled to the 3.3 μm feature. The observed intensity ratio of these two features varies from 0.02 to 0.07. The large uncertainties in the intensities of the 3.45 μm plateau prevent such an accurate determination regarding the degree of its coupling to the other features, but the HD 44179 spectrum suggests that its intensity ratios with the other features vary as well.

As has been discussed in the past (e.g., Russell, Soifer, and Merrill 1977), the fact that the features are resolved and smooth indicates that they are not due to emission lines from atoms or simple gas phase molecules, unless the features are unresolved *Q*-branches. Such an explanation is most plausible for the relatively narrow 3.40 μm feature. However, none of the likeliest simple molecules (CH, CH^+, NH, NH^+) has a *Q*-branch at that wavelength. We conclude, as have others, that the 3.3, 3.4, and 3.45 μm features have other origins.

Previous attempts to explain these and other infrared emission features have been centered on two models. Allamandola, Greenberg, and Norman (1979) proposed that absorption of ultraviolet radiation by molecules in grain mantles leave them in excited vibrational states, which decay by infrared emission. In contrast, Dwek *et al.* (1980) proposed that small grains, which are inefficient infrared emitters except at resonances of bound molecules, become hot enough to emit in the 3 μm and longer wavelength bands. Recently, Sellgren (1984) has suggested that another component of interstellar dust is responsible for the 3.3 μm emission features. In her picture, which has been expanded upon by Léger and Puget (1984), tiny grains, of radius only ~5 Å, are heated by absorption of single UV photons and radiate the energy in the CH stretching modes. Léger and Puget suggest that these grains are actually single large aromatic hydrocarbon molecules. They show a reasonable fit of benzene to the spectral data on NGC 2023 due to Sellgren, Werner, and Dinerstein (1983). The suggested grains are much smaller than those postulated by Dwek *et al.*, and the radiation mechanism is different also; in the Dwek *et al.* picture the small grains reach thermal equilibrium, while the Léger and Puget tiny grains are continuously fluctuating in temperature with each UV-photon absorption. According to Léger and Puget, the cores of these graphite grains are the only small carbon-rich species that can survive the postulated temperature fluctuations without evaporating.

One potential difficulty with the mantle model that should not occur in the model of Léger and Puget concerns the similarity of the 3.3 μm emission features in the diverse objects observed and reported here. Because the material responsible for these features was made *in situ* in NGC 7027 and BD +30°3639 and (probably) HD 44179, and could have been formed in a molecular cloud or as an aggregate from many sources in the case of S106, the identical shapes argue for a very similar emitting material in all cases. Since the formation environments must be different in these various objects, an amorphous material such as a mantle where the detailed composition must vary from object to object would likely show some variation in shape from object to object. Thus, the similar shapes of the 3.3 μm features observed in several objects are more naturally explained in the models of Sellgren and of Léger and Puget, where the emission is from extremely simple, nonamorphous grains which are very nearly identical in all the objects where they are found.

The present observations have several implications with respect to the proposed emission mechanisms. The detailed shapes of the observed features should constrain the chemical composition of the emitting grains. This is particularly true of the aromatic hydrocarbon molecules proposed by Léger and Puget (1984). The differences and similarities among the spectra of the various sources are also significant. We have already discussed how the similar shapes of the 3.3 μm features in the different sources argue for a model in which a single molecule or closely related group of molecules is responsible for this feature in all sources. On the other hand, the varying relative strengths of the different features may require some difference in composition from source to source. Either the 3.3 and 3.4 μm features arise in completely different molecules, or small changes in the responsible molecules or in their binding in the grains must change the relative strengths of the features without altering the shape of the features. In principle, the spectrum of the exciting radiation could also affect the feature strengths if, for example, the 3.4 μm feature requires different energy photons for this excitation than does the 3.3 μm feature.

With respect to the required grain composition, we also note that the Léger and Puget mechanism requires the emitting grains to be formed in a carbon-rich environment. Small hydrocarbon grains could not form in the outflow from an oxygen-rich star. However, they could survive in an oxygen-rich star-formation region such as S106, if they originally formed in the outflow from a carbon star. The composition of the progenitor, and especially its carbon abundance, could have an effect on the strength of the features. Planetary nebulae generally have gas-phase carbon abundances that are about a factor of 2 above solar (French 1982) and thus might be expected to produce stronger features than in the oxygen-rich environments of H II regions. However, in the Léger and Puget model, only a few percent of the total carbon is needed to produce the features in NGC 2023, and therefore the numbers of small grains may not closely follow that carbon abundance.

The above discussion suggests that one might expect to find correlations between the observed spectra and the chemistry and excitation of the different sources. However, such correlations involving the various 3 μm features are not apparent in the present data set. For example, of the two sources showing relatively strong 3.4 μm features, NGC 7027 is a high-excitation planetary nebula, whereas S106 is a much lower excitation H II region. Of those without prominent 3.4 μm features, BD +30°3639 is a low- excitation planetary, and HD 44179 is a rather early–type star. The excitation spectrum of S106 is more like that of BD +30°3639 than NGC 7027, and the grain-formation environment should be most similar in the two planetary nebulae. At present, one can only infer that the newly defined 3.40 and 3.45 μm features are each members of the family of features including those at 3.3, 6.2, 7.7, 8.6, and 11.3 μm, which tend to occur together. Although no correlations are suggested by the present data, in order to clearly establish their absence or presence a much larger sample of sources must be observed in these features at the present spectral resolution or higher.

IV. SUMMARY

Moderate-resolution spectroscopy of NGC 7027, BD +30°3639, IC 418, S106, and HD 44179 from 3.1 to 3.6 μm has shown that the profile of the strong 3.3 μm unidentified emission feature is similar in all five sources. The unidentified feature previously referred to as the 3.4 μm feature actually consists of two components, a low-level emission from 3.35 to 3.60 μm, and a narrow emission peak at 3.40 μm. The strength of the 3.40 μm emission feature relative to that of the 3.3 μm feature varies by a factor of 3 from source to source. The origin and properties of these features may be explained by further development of the small-grain models of Sellgren (1984) and Léger and Puget (1984).

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