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EXCITATION MECHANISMS FOR THE UNIDENTIFIED INFRARED EMISSION FEATURES

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ABSTRACT

We have analyzed infrared and radio observations of various objects to put observational constraints on the mechanism which gives rise to the unidentified emission features at 3.3 μm, 3.4 μm, 6.2 μm, 7.7 μm, 8.6 μm, and 11.3 μm. The results show that gas-grain collisions or fluorescence is not likely to be the excitation mechanism responsible for the observed features. We have reanalyzed thermal emission by dust and conclude that this mechanism can explain the emission features. We have constructed a simple model in which the emission features arise in a population of small, hot, interstellar grains. These grains are very efficient radiators, and the emitting materials only need be a minor grain constituent to provide the power that is emitted in the features. The model offers, therefore, a simple explanation for the absence of these features in absorption.

Subject headings: infrared: sources — molecular processes — nebulae: general

I. INTRODUCTION

One of the major astrophysical problems of low-resolution infrared spectroscopy is the explanation for a series of strong emission features found in the spectra of a variety of bright infrared sources. The features in question, centered at 3.3 μm, 3.4 μm, 6.2 μm, 7.7 μm, 8.6 μm, and 11.3 μm, have thus far eluded satisfactory identification, even though their presence in the spectra of a wide variety of objects shows that the phenomena responsible for these emission features are quite common in astrophysical environments. These unidentified features might be discussed as an interesting astronomical oddity, except for three observational facts. First, they are quite common in the spectra of a variety of nebulae; second, they provide a nonnegligible fraction (several percent) of the total luminosity of these nebulae; and third, the near-infrared luminosity (i.e., $\lambda < 15$ μm) is sometimes dominated by the emission in these features.

In this paper we analyze the observational constraints that can be placed on any emission or excitation mechanism responsible for these features. In Table 1 we summarize many of the observations reported to date of the unidentified emission bands. Here we have included only sources where several of the bands have been unambiguously identified. As can be seen from this table, these bands are found in a wide variety of objects, including planetary nebulae, H II regions, and the nuclei of galaxies. Since the association of the emission features with ultraviolet radiation has been widely discussed, a characteristic temperature for the exciting star(s) of the region is included, where this information is available.

To date, most observations indicate that when seen, the unidentified bands appear together. All the bands are apparently resolved at the resolution available to date ($\Delta\lambda/\lambda \approx 0.01$–$0.02$ in the case of the bands at 6.2 μm and 7.7 μm [e.g., Russell, Soifer, and Willner 1977; Willner *et al.* 1977], $\Delta\lambda/\lambda \approx 0.015$–$0.003$ in the case of the 11.3 μm band [Gillett, Forrest, and Merrill 1973; Bregman and Rank 1975], $\Delta\lambda/\lambda \approx 0.015$–$0.001$ in the case of the 3.3 μm band [Grasdalen and Joyce 1976; Smith *et al.* as quoted by Russell, Soifer, and Merrill 1977]). These observations strongly suggest an emission mechanism associated with solid state resonances in interstellar grains. At first glance, thermal emission from interstellar dust grains is an obvious identification. Thus far, such a mechanism has failed because of a lack of specific candidate materials. Among the common terrestrial minerals, none can satisfactorily match any of the observed bands without predicting another emission band that is not observed. The only exception is the 6.2 μm band, which could be identified as water of hydration in minerals without any contradictory observations. Webster (1980) also suggested that some of the unidentified features may be due to carbyne, but as yet no infrared spectra of this substance are published.

An important observational constraint that any thermal emission model must explain is the absence of

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TABLE 1
SOURCES IN WHICH THE UNIDENTIFIED BANDS ARE FOUND

Source	Type	Observed Bands (μm) 3.3	3.4	6.2	7.7	8.6	11.3	T_* (K)	References
NGC 7027	Planetary nebula	✓	✓	✓	✓	✓	✓	10^5–2×10^5	1, 2, 3
BD+30°3639	Planetary nebula	✓	✓	✓	✓	✓	✓	3×10^4	3, 4, 5
HD 44179	...	✓	✓	✓	✓	✓	✓	10^4	4, 6, 7
Orion Ridge	H II region/ionization front	✓	✓	✓	✓	✓	✓	4×10^4	8, 9, 10
GL 3053	H II region	✓	✓	✓	✓	✓	✓	...	11, 12, 13
GL 437	...	✓	✓	x	x	✓	✓	$<3 \times 10^4$	14
GL 4029	...	✓	✓	✓	✓	✓	✓	...	15
NGC 253	Galaxy nucleus	✓	✓	x	x	✓	✓	...	4, 16
M82	Galaxy nucleus	✓	✓	✓	✓	✓	✓	3×10^4	16, 17

NOTES.—✓ = observed in spectrum. x = no observations available.

REFERENCES.—(1) Merrill *et al.* 1975. (2) Russell, Soifer, and Willner 1977. (3) Gillett *et al.* 1973. (4) Russell, Soifer, and Merrill 1977. (5) Russell *et al.* 1980. (6) Russell *et al.* 1978. (7) Cohen *et al.* 1975. (8) Sellgren 1980. (9) Soifer *et al.* 1980. (10) Aitken *et al.* 1979. (11) Gillett and Merrill 1978. (12) Russell 1979. (13) Merrill 1977. (14) Kleinmann *et al.* 1977. (15) Willner *et al.* 1980. (16) Gillett *et al.* 1975. (17) Willner *et al.* 1977.

these bands in absorption. Many protostellar infrared sources are viewed through very large column densities of cold intervening material (Merrill, Russell, and Soifer 1976; Soifer *et al.* 1979), and yet no evidence for absorption in these bands has been found in the spectrum of any compact infrared source.

This lack of a satisfactory identification based on thermal emission of solids has lead to other suggested mechanisms, the most prominent being fluorescence emission in solids (Gillett 1977). Observationally, the unidentified bands have been found only when there is known to be a large flux of UV photons present which could be responsible for exciting the fluorescence. Based on this correlation, Allamandola and Norman (1978*a*, *b*) and Allamandola, Greenberg, and Norman (1979, hereafter AGN) have noted the correspondence in wavelength between the features and vibrational transitions in simple molecules, and they identified the bands as fluorescence emission from molecular impurities in mantles on interstellar grains. While this is qualitatively an attractive model, it is shown below through analysis of the observations that this mechanism is unlikely to explain the emission bands.

To pursue a quantitative analysis of the emission bands, we have taken as examples four sources where the bands are found, NGC 7027, BD+30°3639, HD 44179, and M82, for detailed analysis. All of these objects show the emission bands quite prominently in their infrared spectra. NGC 7027 and BD+30°3639 are planetary nebulae with central star temperatures of 1–2×10^5 K and 3×10^4 K, respectively. HD 44179 is a binary system submerged in a thick circumstellar dust shell. The temperature of the stars is $\sim 10^4$ K. The luminosity source of the nucleus of the galaxy M82 is thought to be stellar with a temperature of $\sim 3 \times 10^4$ K.

II. GENERAL EXCITATION MECHANISMS

Two of the mechanisms proposed to excite the resonances in the grains that give rise to the emission bands are: (1) collisions between the grains and gas-phase atoms or molecules and (2) the absorption of visual-ultraviolet (V-UV) photons. To quantify the discussion of these mechanisms, we consider the total intensity I_λ in the line at wavelength λ and write it in terms of the collision rate $R(i)$ (in s^{-1}) due to the excitation mechanism (i) as

$$I_\lambda = F_\lambda \Delta\lambda = E_\lambda R(i)\alpha(i)/(4\pi d^2) , \qquad (1)$$

where F_λ is the observed flux, $\Delta\lambda$ the line width, E_λ the energy of a photon at wavelength λ, $\alpha(i)$ the efficiency at which the particle (gas atom or molecule, V-UV photon) colliding with the grain is converted into a fluorescence photon, and d is the distance to the source. In this equation, and all following ones, the units are cgs unless noted otherwise. Our purpose is to estimate the efficiency of the various excitation mechanisms and hence assess their likelihood of explaining the emission bands. We confine our discussion to processes in which each collision produces only one infrared photon.

Our general approach is to calculate the collision rate R from associated observable effects of the relevant excitation mechanism. The advantage of our approach is that the excitation efficiency is derived from observational data alone and therefore does not depend on assumed nebular parameters or distances. The collision rate with ambient particles in the ionized gas can be calculated from the free-free emission rate,

TABLE 2
NEBULAR PARAMETERS

Object	F_{IR} (W cm^{-2})	S_ν (Jy)	ν (GHz)
NGC 7027	2.4×10^{-14} [a]	5.86[e]	10
BD+30°3639	5.4×10^{-15} [b]	0.477[e]	10
HD 44179	2.3×10^{-14} [c]	no radio continuum[g]	
M82	9.3×10^{-15} [d]	0.6[f]	86

[a] Telesco and Harper 1977.
[b] Moseley 1980.
[c] Kleinmann *et al.* 1978.
[d] Telesco and Harper 1980.
[e] Cohen and Barlow 1974.
[f] Kellermann and Pauliny-Toth 1971.
[g] Cohen *et al.* 1975.

inferred from radio observations. The absorption rate of V-UV photons can be derived from the observed continuum infrared flux F_{IR}, because the sources under consideration emit the bulk of their luminosity in the infrared.

The observational data that were used to set upper limits on the collision rate R are summarized in Table 2 for the various objects considered in this paper. With these upper limits, we estimate the minimum required efficiency of the proposed excitation mechanisms.

a) *Collisional Excitation Mechanisms*

The collision rate between a gas species and a grain is given by $R_s = n_s n_{gr} \sigma_{gr} v_s V$, where n_s is the number density of the relevant gas species, v_s its thermal velocity, n_{gr} is the grain number density, σ_{gr} its geometrical cross section, and V is the volume of the emitting region. In an ionized plasma collisions with electrons occur more frequently than collisions with any other gas species. Excitation by electron collisions is therefore potentially the most efficient collisional excitation mechanism. The plasma also gives rise to free-free emission at a rate (Spitzer 1978)

$$J_\nu = 6.8 \times 10^{-38} n_e n_i T^{-1/2} g_\nu \, \text{ergs cm}^{-3}\,\text{s}^{-1}\,\text{Hz}^{-1}, \quad (2)$$

where n_e and n_i are, respectively, the electron and ion number densities, T the temperature of the gas, and g_ν a factor which is about 4 for the frequencies considered in this paper. Expressing the electron collision rate in terms of J_ν for typical nebular temperatures and gas-to-dust mass ratios (i.e., $T = 10^4$ K and $n_{gr}\sigma_{gr} = 8 \times 10^{-22} n_H$, where n_H is the hydrogen number density), we get that α_{coll}, the efficiency factor for excitation by electron-grain collisions, is given in terms of the observable quantities only:

$$\alpha_{coll} = 4 \times 10^{16} \frac{\Delta\lambda(\mu\text{m})}{E_\lambda(\text{eV})} \frac{F_\lambda(\text{W cm}^{-2}\,\mu\text{m}^{-1})}{S_\nu(\text{Jy})}, \quad (3)$$

where S_ν is the observed radio continuum flux, assumed to be optically thin, at frequency ν in units of Jy($=10^{-26}$ W m^{-2} Hz^{-1}). Table 3 lists the value of α_{coll} for various nebulae and emission bands. The results show that the required efficiency is significantly larger than unity in most cases. We therefore conclude that collisions with electrons or gas-phase ions are very unlikely excitation mechanisms of the observed bands. Collisions in the surrounding neutral material are even less likely, since they involve heavier species with temperatures that are significantly lower than those of the H II region.

The efficiencies listed in Table 3 do not include the effects of grain charge. The effective cross section of the grains will be increased if they are positively charged; this may be the case if photoemission from the grains is important and if the gas density is sufficiently low. For the types of objects under consideration here the cross section might be increased by a factor of 5 by this process (Draine and Salpeter 1979), but the required efficiencies are still greater than unity in most cases.

TABLE 3

COLLISIONAL EXCITATION EFFICIENCIES IN VARIOUS NEBULAE[a]

WAVELENGTH (μm)	α_{coll}		
	NGC 7027	BD+30°3639	M82
3.3	0.54	1.5	3.2
6.2	3.4	9.2	19.9
7.7	14.9	36.7	90.8
8.6	4.4	9.0	16.6
11.3	9.3	16.0	14.5

[a] Calculated for electron collisions.

b) *Ultraviolet Fluorescence*

The fluorescence efficiency has been estimated from the observational data by comparing the number of photons emitted in the various bands to the number of exciting photons emitted by the source. The fluorescence efficiency can be written as

$$\alpha_{ph} = \frac{E_{\lambda_{UV}} F_\lambda(\text{W cm}^{-2}\,\mu\text{m}^{-1})\Delta\lambda(\mu\text{m})}{E_\lambda F_{IR}(\text{W cm}^{-2})}, \quad (4)$$

where $E_{\lambda_{UV}}$ represents a mean energy of the V-UV photons emitted by the source. Total infrared fluxes F_{IR} from the various sources are given in Table 2, and in Table 4 we list the observed fluxes F_λ for the various bands, the band widths $\Delta\lambda$, the energy of the emitted photons E_λ, and the derived value of α_{ph} for the various bands in the different sources. In the calculations, we took $E_{\lambda_{UV}} = 10$ eV, which is consistent with the temperature of the exciting stars. A smaller value of $E_{\lambda_{UV}}$ would increase the number of exciting photons and correspondingly decrease the required excitation efficiency. However, from the results of Table 4 we see that a decrease by a factor of $\sim$2–3 in the required efficiency will not change our conclusions. The table shows that the 3.3 μm band can be attributed to fluorescence in dust, since the required efficiency is reasonably low. Other bands, however, require excitation efficiencies which are comparable to unity. Although, in principle, an incident UV photon may give rise to more than one fluorescence photon, we feel that a value of α_{ph} which is about unity is unacceptably high, since we have already made the generous assumption that all the luminosity of the exciting star is emitted in photons that induce fluorescence. Other mechanisms are therefore needed to excite these bands. However, the idea of invoking more than one excitation mechanism as an explanation of the emission bands is unattractive, since all the features appear together in the sources observed to date. We therefore conclude that fluorescence is an unlikely excitation mechanism for the bands.

Our conclusions contradict those reached by AGN, who calculated the efficiency for the conversion of a

TABLE 4

PHOTON EXCITATION EFFICIENCIES α_{ph}, CALCULATED FROM OBSERVED FEATURES IN VARIOUS NEBULAE[a]

			NGC 7027		BD+30°3639		HD 44179		M82	
WAVELENGTH (μm)	ENERGY (eV)	OBSERVED WIDTH (μm)	F_λ (W cm^{-2} μm^{-1})	α_{ph}	F_λ (W cm^{-2} μm^{-1})	α_{ph}	F_λ (W cm^{-2} μm^{-1})	α_{ph}	F_λ (W cm^{-2} μm^{-1})	α_{ph}
3.3.........	0.38	0.1[b]	3×10^{-16}	0.03	7×10^{-17}	0.03	0.7×10^{-15}	0.08	1.8×10^{-16}	0.05
6.2.........	0.20	0.2	5×10^{-16}	0.21	1.1×10^{-16}	0.20	1.0×10^{-15}	0.43	3.0×10^{-16}	0.32
7.7.........	0.16	0.5	7×10^{-16}	0.90	1.4×10^{-16}	0.80	1.2×10^{-15}	1.62	4.4×10^{-16}	1.47
8.6.........	0.14	0.3	3×10^{-16}	0.26	5×10^{-17}	0.19	4.0×10^{-16}	0.36	1.2×10^{-16}	0.27
11.3.........	0.11	0.3	5×10^{-16}	0.57	7×10^{-17}	0.35	3.0×10^{-16}	0.36	8.0×10^{-17}	0.23
Total efficiency..................................				1.97		1.59		2.84		2.34

[a] Fluxes are from the references given in Table 1, with the continuum subtracted. No correction for extinction has been made to the observed fluxes.

[b] The observed width here includes the 3.4 μm feature.

UV photon to a fluorescence photon and found it to be only a few percent. They calculated the fluorescence efficiency, α_{ph}, by comparing the total number of UV photons emitted by the exciting stars, which are represented by blackbodies with a given effective radius and temperature, to the total number of fluorescence photons which, for a given observed flux, depends on the distance to the source. In their calculations, AGN took this distance to be only 100 pc. Their calculated efficiencies should therefore be multiplied by a factor of $(10\,d)^2$, where d is the actual distance to the source in kpc. The distance to NGC 7027, for example, is estimated to be between 0.5 and 1.77 kpc (O'Dell 1962; Cudworth 1974). So, applied to this source, their calculated efficiencies should be multiplied by a factor of $\sim$30–300, giving a value that is consistent with our estimates.

III. THERMAL EMISSION FROM DUST

Thermal emission by dust grains has been rejected as a likely mechanism for the emission bands, because of the lack of specific candidate materials and the absence of these bands in absorption. The difficulties we find with the other proposed mechanisms lead us to reexamine the thermal emission mechanism and to explore its observational consequences. The absence of these bands in absorption leads us to consider the possibility that the resonances exist only in a population of small grains. In the vicinity of an exciting star, these small grains can attain higher temperatures than large grains, making them very efficient radiators in the various emission bands. Consequently, only a small amount of emitting material needs to be present in the small grains to provide the power radiated in these bands, offering a simple explanation for their absence in absorption. Qualitatively, in the region of a UV source the amount of energy absorbed, and then reemitted in the infrared, will be proportional to the cross-sectional area of the grains, or $\tau_{UV} \propto na^2$. In the infrared, the energy absorbed will be proportional to the mass of the grains, or $\tau_{IR} \propto na^3$. The ratio of infrared to UV absorption is then $\tau_{IR}/\tau_{UV} \propto a$. For a bimodal population of large (1) and small (2) grains, this implies

$$[\tau_{IR}(1)/\tau_{UV}(1)]/[\tau_{IR}(2)/\tau_{UV}(2)] = a_1/a_2,$$

or

$$\tau_{IR}(2)/\tau_{IR}(1) = (a_2/a_1)[\tau_{UV}(2)/\tau_{UV}(1)].$$

Thus, even if the small grains absorb a significant fraction of the UV radiation which is then reemitted in the infrared in the unidentified features, absorption features in the infrared need not appear, since the absorption of the large grains can still dominate the infrared absorption spectra. Specifically, if $a_2/a_1 \approx 0.10$ and $\tau_{UV}(2)/\tau_{UV}(1) \approx 0.10$, then 10% of the energy emitted in the infrared near a UV source would appear in the unidentified emission features, while in absorption toward an infrared source, the same bands would appear at only 1% of the strength of the bands in the large grains. In the following, we will develop this idea on a more quantitative basis from independent observations that indicate the presence of small, hot grains in the Orion ionization front in which the unidentified features are strong (Aitken *et al.* 1979; Soifer *et al.* 1980; Sellgren 1980).

Infrared studies of the ionization front in the Orion nebula (Becklin *et al.* 1976) indicate that the infrared flux from this ridge is due to emission from grains with a range of temperatures. This temperature range was attributed by Becklin *et al.* (1976) to a distribution of grain sizes. The infrared energy distributions of other sources in Table 1 are also consistent with a range of grain temperatures (see, e.g., Telesco and Harper 1977, for NGC 7027). However, the favorable geometry of the Orion ionization front and the fact that the emission comes from outside of the ionized gas makes it particularly straightforward to relate the temperature distribution to a size distribution in this case (cf. Becklin *et al.* 1976). Assuming a bimodal distribution of grain sizes, they found that the observed infrared spectrum is consistent with the larger grains having a temperature of 60 K and the smaller grains having a temperature of 300 K. For a given ambient radiation field, the temperature of a dust grain is determined by the ratio of its emissivity at short wavelengths, where the energy is absorbed, to its emissivity at longer wavelengths, where the energy is radiated away. To show that the ideas under consideration are plausible, we adopt an idealized model in which the effects of the bands on the grain temperature are ignored and in which the emissivity of a grain is equal to unity up to a wavelength $\lambda = 2\pi a$ and decreases as λ^{-k} at longer wavelengths, where a is the radius of the grain. The Orion observations can then be reproduced if the hotter grains have sizes between 0.005 and 0.01 μm for an emissivity that decreases as λ^{-2}, whereas the cooler grains have a size of $a \approx 0.1$ μm for an emissivity that decreases as λ^{-1}. These values of the sizes and emissivities were chosen to be consistent with the grain properties assumed by Becklin *et al.* (1976), who chose those of silicates for the large grains and those of graphite for the small grains.

The total power emitted by a single grain is given by

$$L_{gr} = 1.2 \times 10^{-14} a^3(\mu\text{m}) T_{gr}{}^5 \text{ ergs s}^{-1}\,, \qquad (5)$$

for the large grains, and by

$$L_{gr} = 2.5 \times 10^{-17}\, a^4(\mu\text{m}) T_{gr}{}^6 \text{ ergs s}^{-1}\,, \qquad (6)$$

for the small grains, where T_{gr} is the grain temperature.

The total power absorbed by a grain in a radiation field of temperature T_* is

$$P = 4\pi a^2 \sigma T_*{}^4 Q(k, x) W\,, \qquad (7)$$

where

$$Q(k, x) = 1 - \frac{15}{\pi^4}\left(\int_0^x \frac{t^3 dt}{e^t - 1} - x^{-k}\int_0^x \frac{t^{3+k}dt}{e^t - 1}\right), \qquad (8)$$

with $k = 1$ for the large grains, and $k = 2$ for the small grains, and where $x = 1.44 \times 10^4/[2\pi a(\mu\text{m})T_*]$. W is a geometric dilution factor determined by the distance from the grain to the star. The relative numbers of small and large grains can be derived from the ratio of the power absorbed by the two grain populations from the radiation field and observed as reemission in the infrared. The total infrared luminosity emitted by the large grains is 6000 $L_\odot$, and that emitted by the small grains is 500 $L_\odot$. This gives

$$\frac{n_2}{n_1} = 0.08\left(\frac{a_1}{a_2}\right)^2 \frac{Q(1, x_1)}{Q(2, x_2)}\,, \qquad (9)$$

where n_1 and n_2 are the number density of large and small grains, respectively, and a_1 and a_2 are their radii. For a ratio of a_1/a_2 between 10 and 20, and assuming $T_* = 40{,}000$ K for the Trapezium stars, the corresponding values of n_2/n_1 are between 20 and 200.

In the following it is argued that the unidentified emission bands can be due to thermal emission from the hot, small grains with resonances at the observed wavelengths, whereas the larger, cool grains are responsible for the observed absorption features like the 10 μm silicate band. The power emitted by a grain due to a resonance centered around the frequency ν_0, with a resonance width δ is given by

$$L_{\nu_0} = 4\pi a^2 \int_{\nu_0-\delta/2}^{\nu_0+\delta/2} \pi B_\nu(T_{gr}) Q_\nu d\nu\,, \qquad (10)$$

where B_ν is the Planck function and T_{gr} the grain temperature. The emissivity Q_ν is sharply peaked around ν_0, and equation (10) can be integrated to give (Field 1969)

$$L_{\nu_0} = 4\pi^2 a^2 B_{\nu_0}(T_{gr}) \int_{\nu_0-\delta/2}^{\nu_0+\delta/2} Q_\nu d\nu = \frac{16\pi^3 a^3 N e^2 f_0}{3Mc} B_{\nu_0}(T_{gr})\,, \qquad (11)$$

where N is the number density of oscillators in the grain, f_0 their oscillator strength, and M their mass. For $h\nu_0 \gg kT_{gr}$, equation (11) can be written as

$$L_{\nu_0} = 3.3 \times 10^4 \left(\frac{a}{\lambda_0}\right)^3 e^{-x_0} \frac{\tilde{f}}{A} \text{ ergs s}^{-1}\,, \qquad (12)$$

where $x_0 = 1.44 \times 10^4/(\lambda_0(\mu\text{m})T_{gr})$, A is the oscillator mass in atomic mass units, and N was normalized to the number density of graphite ($N_{\text{graphite}} = 1.1 \times 10^{23}$ cm^{-3}). The parameter $\tilde{f}$, therefore, is the product of the oscillator strength times the number density of oscillators in the grain relative to the density of graphite.

The factor $\tilde{f}/A$ can be calculated from the observed ratio of the emissivity in the line to that in the continuum. The emissivity in the line ν_0, averaged over the band, is given by

$$Q_{\nu_0} = \frac{1}{\delta}\int_{\nu_0-\delta/2}^{\nu_0+\delta/2} Q_\nu d\nu = 7.1 \times 10^7 \frac{a\lambda_0{}^2}{\Delta\lambda_0}\frac{\tilde{f}}{A} \text{ (cgs units)}\,. \qquad (13)$$

Using our prescription for the small grain emissivity, we find that the ratio of the emissivity in the line to that in the continuum, $Q_{\nu_0}{}^c$, is given by

$$Q_{\nu_0}/Q_{\nu_0}{}^c = 1.8 \times 10^6 \frac{a\lambda_0{}^2}{\Delta\lambda_0}\frac{\tilde{f}}{A} \text{ (cgs units)}\,. \qquad (14)$$

Observations of the 3.3 μm band in the Orion ridge show that the line-to-continuum ratio is larger than ~ 7, requiring $\tilde{f}/A \gtrsim 1.7 \times 10^{-3}$. The factor $\tilde{f}/A$ can also be calculated from the observed fraction of the total luminosity of the small grains that is emitted in the line. Observations of the Orion ridge (Sellgren 1980) show that about 5×10^{-3} of the luminosity of the small grains, which have $T \approx 300$ K, is emitted in the 3.3 μm band. Calculating the ratio L_{ν_0}/L_{gr} from equations (6) and (12), we find a similar value of $\tilde{f}/A \approx 2 \times 10^{-3}$. Similar calculations for the other bands give even smaller values for $\tilde{f}/A$. The smallness of the factor $\tilde{f}/A$ is reassuring, because it shows that the materials which produce the unidentified bands need not be the dominant constituents of the interstellar dust and that modest values for the intrinsic strengths of the bands are acceptable.

The lack of the emission features in absorption can be now understood by comparing κ, the optical depth per unit length due to a given band, with that of the 10 μm silicate feature. The absorption cross section at wavelength λ_0, averaged over the band, is given by

$$C_{\lambda_0} = \pi a^2 Q_{\nu_0} = 5.3 \times 10^7 V_{\rm gr} \frac{\lambda_0^{\;2}}{\Delta\lambda_0} \frac{\tilde{f}}{A} (\text{cgs units}) , \quad (15)$$

where $V_{\rm gr}$ is the volume of the grain. For the 3.3 μm feature, $\tilde{f}/A$ was estimated to be $\sim 2 \times 10^{-3}$, so that $C_{3.3\,\mu\rm m} = 1.1 \times 10^3 V_{\rm gr}\,\rm cm^2$. Taking a density of 3 g cm^{-3}, and a silicate mass absorption coefficient of $3 \times 10^3\,\rm cm^2\,g^{-1}$ (Friedmann, Gürtler, and Dorschner 1979), we find that $C_{10\,\mu\rm m} = 9 \times 10^3\, V_{\rm gr}\,\rm cm^2$. If the silicate band is assumed to arise from the large grain population, and the relative numbers and sizes of large and small grains are the same everywhere as are found in the Orion ridge, then using the relation $\kappa_{\lambda_0} = nC_{\lambda_0}$, we find

$$\kappa_{3.3\,\mu\rm m} = 0.13 \left(\frac{n_2}{n_1}\right)\left(\frac{a_2}{a_1}\right)^3 \kappa_{10\,\mu\rm m}$$
$$\approx 3 \times 10^{-3} \kappa_{10\,\mu\rm m} , \quad (16)$$

for $a_1/a_2 = 10$–20 and $n_2/n_1 = 20$–200. The absorption coefficients, relative to the silicate band, are even smaller for the other unidentified bands, and so these bands are also unobservable in absorption.

The basic ideas of the model may be summarized as follows. The small grains attain high temperatures when exposed to a strong UV radiation field, so that appreciable amounts of energy are emitted in the unidentified bands. Since the infrared cross section scales as grain volume, while the UV cross section scales as grain area, the unidentified bands are absent in absorption even though they are prominent in emission.

The strongest argument in favor of the fluorescence model for the emission bands is the association of the bands with UV sources. In our calculations we showed, however, that the UV sources probably do not emit enough photons to produce the observed emission by fluorescence. The association with UV sources is therefore not related to the fluorescence phenomena, but to the availability of UV photons required to heat the small grains. The power emitted in the bands is a rapidly increasing function of grain temperature (see eq. [12]), which for a fixed stellar luminosity depends on the radius of the grain, its distance from the star, and the star's effective surface temperature. In Table 5 we calculated the temperature attained by a population of small ($a = 0.01\ \mu$m) and large ($a = 0.1\ \mu$m) grains placed at a distance of 10^{18} cm from an exciting star with a fixed luminosity of $L = 4 \times 10^5\, L_\odot$, for various values of T_*, the effective stellar surface temperature. The results show that the small grains can attain high temperatures which increase rapidly with

TABLE 5

GRAIN TEMPERATURE $T_{\rm gr}$ VERSUS EFFECTIVE STELLAR TEMPERATURE T_*[a]

T_* (K)	$T_{\rm gr}$ (K) $a = 0.1\ \mu$m	$T_{\rm gr}$ (K) $a = 0.01\ \mu$m
4×10^4	80	300
3×10^4	80	280
2×10^4	80	240
1×10^4	78	190
6×10^3	76	160

[a] For grains at a distance of 10^{18} cm, and a stellar luminosity of $4 \times 10^5\, L_\odot$.

T_*, whereas the large grains attain considerably lower temperatures which do not depend on the effective temperature of the exciting star. The table demonstrates that both the absolute and relative amounts of power emitted by the small grains are sensitive functions of stellar temperature, so that the unidentified bands are naturally strongest in the vicinity of UV sources.

A thermal emission model predicts that the ratio between the fluxes emitted in the various bands depends, for a given, relative, intrinsic line strength, only on the grain temperature. We therefore subjected our model to an observational test in which we assumed that the small grain population in each source can be characterized by a single temperature. Different relative flux ratios in the various sources are then attributed to different grain temperatures. A χ^2-fitting routine was used to determine the grain temperature in the various sources listed in Table 4. The grain temperatures were restricted to the range 200–2000 K, which represent limits of brightness temperature for the observed fluxes and melting temperatures for the grains, respectively. We also assumed that the emissivity of the grains as a function of wavelength is the same in each source. The resulting fit was found to be poor, demonstrating that the differences in the relative flux ratios in the various sources cannot be attributed only to differences in grain temperatures. For example, the ratio $F_{7.7}/F_{11.3}$ of the flux emitted in the 7.7 μm band to that emitted in the 11.3 μm band varies by a factor of ~ 4.5 between the different sources. This cannot be produced by variations in temperature for temperatures between 200 and 2000 K and requires changes in the ratio of intrinsic line strength. The flux ratio $F_{7.7}/F_{3.3}$, on the other hand, is extremely sensitive to grain temperature, but varies by only a factor of ~ 1.7 in the various sources. We interpret the results of our model as showing that if our assumption of an isothermal grain population in the emitting region is correct, then the temperature of the grains in this region is virtually identical for the sources considered, and the intrinsic strengths of the emission features vary by factors of ~ 2–4 from source to source. The variation in emission strengths makes a single emitting material unlikely and suggests that the features are due to a group of different materials which occur naturally together and whose relative abundances vary from source to source. The narrow range of effective source temperatures may be due to the nature of the emitting material, as explained in § IV.

IV. SPECULATIONS AND CONCLUSIONS

The analysis of § II strongly argues against the nonthermal emission mechanisms considered for the unidentified bands. The fluorescence mechanism of § II*b* cannot be ruled out, since it is energetically possible; however, we feel that the efficiency required is large enough to make this improbable. However, in a thermal emission model, one is still left with the problem of positively identifying the substance(s) which produce the emission features. It was argued in § III that the source of the emission bands is small ($\lesssim 0.01$ μm) and hot (~ 300 K) grains. The existence of these small hot grains in the Orion ridge, where the unidentified bands are prominent, is suggested by the continuum infrared energy distribution (Becklin *et al.* 1976), and the interstellar medium in general is believed to contain a population of small grains, on the basis of the UV extinction (Aannestad and Purcell 1973, and references therein).

We found from the small variations of the observed flux ratios from source to source that the unidentified features arise in materials which emit over a very narrow range of temperatures. This suggests that the emitting material is a volatile mantle on the small grains. Since the amount of thermal emission for the temperatures and wavelengths involved is very sensitive to temperature, the mantle does not radiate significantly when the grain is cold. When the mantle is exposed to UV radiation near an exciting star, it becomes hot enough to emit the features, but at a slightly higher temperature, it evaporates. This picture is consistent with observations of the Orion nebula at 3.3 μm and 11.3 μm (Sellgren 1980; Aitken *et al.* 1979), which show that the unidentified emission comes from the interface of the H II region and the surrounding neutral material, but is absent in the H II region itself.

One possibility is that the seed grains on which these mantles form are graphite, since small graphite grains are the most likely candidates for producing the 2200 Å extinction feature (Gilra 1972). This feature is present, though weak, in the Orion nebula (Bless and Savage 1972). Thus, if the mantles form on graphite, the features would be seen in both oxygen-rich environments, such as the Orion nebula, and carbon-rich environments, such as NGC 7027. If the initial layers of the mantle are formed by chemical reactions between incident atoms and the grain surface, rather than by simply coating the grains with molecules, these layers would naturally form carbon-rich ices independent of the C/O ratio of the region. This is an attractive possibility, since the 3.3 μm band is coincident with the C–H stretching mode, and the 7.7 μm band with an H–C–H bending mode, as was first pointed out by Allamandola and Norman (1978*a*). They also noted that the 6.2 μm and 11.3 μm bands coincide in wavelength with features of H_2O, which, together with the observed small variations in band strengths from source to source, suggests a mixture of ices in the mantle. It is possible that the mantle is a complex mixture of polymerized ices, like the "oily plastics" suggested by Salpeter (1977). These identifications are highly tentative and desperately need further investigation. Any possible identification must also take into consideration small particle effects, which for grains as small as the ones discussed here can shift resonance wavelengths by significant amounts (Huffmann 1977).

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