Modelling the ice band towards HD 29647

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Summary. Calculations have been made on a core–mantle–mantle grain model whose outer mantle consists of dirty ice material accreted in a molecular cloud. The theoretical predictions of both the strength and shape of the H_2O band are consistent with infrared observations of HD 29647. It is shown that the absence of a 2200 Å hump cannot be caused by mantles on small graphite particles and therefore must be due to a real depletion of the hump carrier.

1 Introduction

Observations of HD 29647 show an anomalously weak 2200 Å extinction hump (Snow & Seab 1980; Seab, Snow & Joseph 1981). Earlier observations of the diffuse interstellar bands in this star (Snow 1973) showed the strengths of these bands to be relatively weak with respect to the rather large colour excess $E(B-V)$ of 1.00 (Crutcher 1980). This is presumed to indicate the presence of grains larger than those characteristic of diffuse interstellar clouds (Snow & Cohen 1974). Large grains are also implied by the rather large value $R = 3.5$ for the ratio of total to selective extinction (Whittet *et al.* 1981).

A suggested explanation of the absence of the 2200 Å hump is that the graphite grains, which are thought to be responsible for this extinction feature, are coated with a dirty ice mantle, which hides the 2200 Å hump (Snow & Seab 1980). If so, there should be an appreciable 3 μm absorption band in the infrared, due to the H_2O in the mantle. To test this hypothesis Whittet *et al.* (1981) and also Goebel (1983) made observations in the infrared. The conclusion of the former was there is no such ice band in HD 29647, whereas the latter measured a dip of $0^m.1$ at 3.10 μm.

The purpose of this paper is to show from a theoretical point of view that the observations of Whittet *et al.* are consistent with the presence of an ice band due to a mantle and that the dip of $0^m.1$ measured by Goebel is what we expect according to our grain model. Furthermore, we perform Mie theory calculations of coated graphite grains to show whether a reasonable thickness of dirty ice mantle can eliminate the 2200 Å extinction hump.

2 A grain-mantle model for the ice band in HD 29647

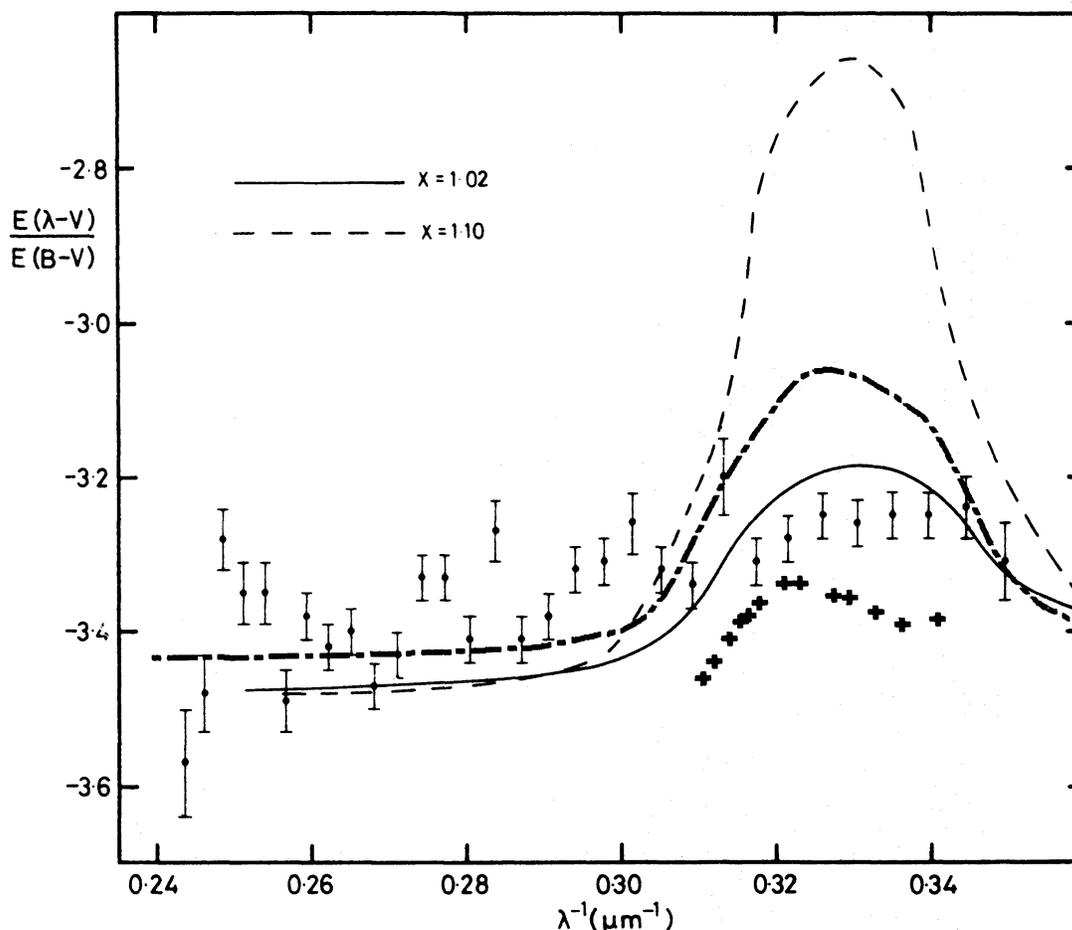Whittet *et al.* (1981) derived a value of $R = 3.5 \pm 0.1$ for the ratio of total to selective

Figure 1. Spectrum for HD 29647 and comparison with silicate core—ice mantle particles according to Whittet *et al.* (1981) for different ratios, x, of mantle to core radius, where $a_c = 0.2\,\mu$m. Included in this figure are the observations + + + by Goebel (1983), as derived from his fig. 2, the vertical scale for this being arbitrarily displaced; also shown are correct Mie theory calculations — — — - — using Whittet's grain model with $x = 1.10$ and Legér *et al.* ice.

extinction from broad band measurements of HD 29647, using $E(B-V) = 1.00$ and a spectral type B8V. Straizys, Wisniewsky & Lebofski (1982a), using somewhat different assumptions, i.e. $E(B-V) = 1.07$ and, as classification, a peculiar mercury—manganese star of type Bp5III, also derive a value of $R = 3.5$. Since the so-called normal extinction curve for the general interstellar medium is characterized by $R = 3.1$ (Savage & Mathis 1979) we are dealing with larger grain sizes. The infrared observations of Whittet *et al.* are shown in Fig. 1, where the value of $E(\lambda-V)/E(B-V)$ is seen to approach a value between 3.4 and 3.5 as λ increases.

We represent the normal interstellar grain as consisting of a 0.05 μm silicate core with a mantle of organic refractory material of 0.12 μm outer radius, which has evolved from photoprocessing of ices (Greenberg 1982). This is a model for a diffuse cloud grain which has no H_2O ice band, even though it contains a substantial amount of oxygen. Such a grain can accrete an extra mantle within a cloud. The extra grain mantle normally contains a large fraction of H_2O along with other molecules. For example, from observations of protostellar sources, and in particular the BN source, one can deduce this fraction to be about 60 per cent (Greenberg 1982). A theoretical calculation of gas plus grain-mantle chemistry by
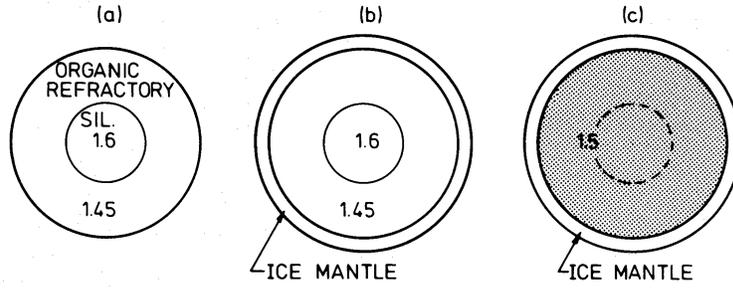
Figure 2. Schematic core—mantle grains: (a) diffuse cloud grain consisting of a silicate core and an organic refractory mantle; (b) molecular cloud grain consisting of the diffuse cloud grain with an accreted ice mantle of radius $a_m = a_2$; (c) molecular cloud grain for which the core plus organic refractory mantle is represented by a compound core of radius $a_{cc} = a_1$ with averaged index of refraction.

d'Hendecourt, Allamandola & Greenberg (1984) also seems to lead to a preponderance of H_2O in the mantle. In no case, however, can one assume that by normal cloud accretion a pure H_2O ice mantle will form. Consequently we shall use in our model a mantle either of pure H_2O or of a mixture for which we have measured optical constants namely, $H_2O : NH_3 = 3 : 1$ (Hagen, Tielens & Greenberg 1983; Greenberg, van de Bult & Allamandola 1983). The outer ice-containing mantle is estimated to be about 10 per cent larger in radius than the inner mantle.

In Fig. 2 we show the schematic grain model. The silicate core radius is a_c and its index of refraction m_c is taken to be 1.6 in the spectral region of interest. In the molecular cloud the combined silicate core—organic refractory mantle ($m_{OR} \sim 1.45$) is represented by a large compound core of the same radius a_1 as the organic refractory mantle, but with a mean index of refraction of the compound particle, $m_1 = 1.5$. This mean can be demonstrated by phase shift averaging assuming $a_c = 0.05\ \mu m$ and $a_m = a_1 = 0.12\ \mu m$. The outer ice-containing mantle has a radius a_2 and the indices of refraction are as measured in our laboratory. The dielectric coefficient of the outer mantle is defined by $\epsilon = \epsilon_1 - i\,\epsilon_2 \equiv m_2^2$, where $m_2 = m_2' - i\,m_2''$ and $\epsilon_1 = m_2'^2 - m_2''^2$, $\epsilon_2 = 2m_2'm_2''$.

Although detailed computations will be obtained using Mie theory calculations it is instructive for determining the trends produced by varying the size and optical properties to estimate the band strengths from a modified Rayleigh approximation for spheres:

The absorption cross-section for a particle whose size is small with respect to the wavelength, as is the case here, and which consists of a core—mantle in which only the mantle absorbs, is given by:

$$C_{abs}(\lambda) = -4\pi k\ \text{Im}\ (\alpha),$$

where $k = 2\pi/\lambda$ and where the polarizability α in this approximation is given by:

$$\alpha = \frac{3}{4\pi}\ \frac{m_2^2 - 1}{m_2^2 + 2}\ V_{mantle}, \tag{1}$$

in which V_{mantle} is the volume of the mantle. This results in:

$$C_{abs}(\lambda) = -4\pi k \cdot (a_2^3 - a_1^3)\ \text{Im}\ \frac{m_2^2 - 1}{m_2^2 + 2} = 12\pi k\,(a_2^3 - a_1^3)\ \frac{\epsilon_2}{(\epsilon_1 + 2)^2 + \epsilon_2^2}, \tag{2}$$

where a_2 is the characteristic or mean size corresponding to the correct wavelength dependence of visual extinction. Thus the ratio of absorption in the infrared to the visual extinction is given by $A_{abs}(\lambda)/A_V \equiv C_{abs}(\lambda)/C_V$, with $A_{abs}(\lambda)$ and A_V the absorptions in the infrared
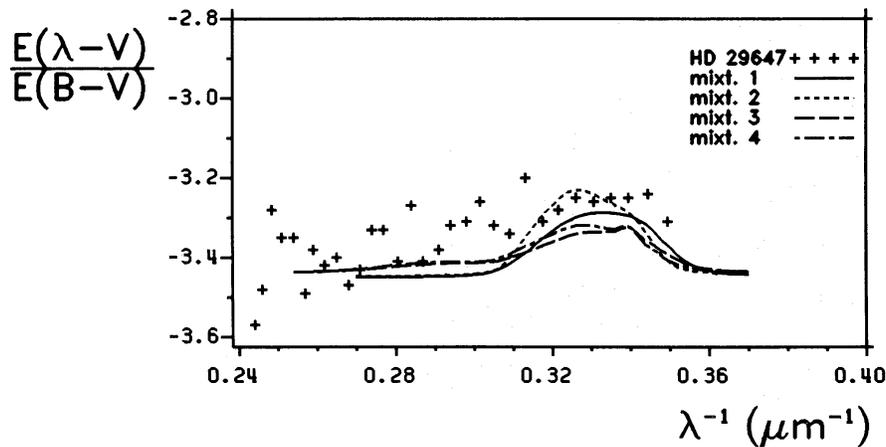
Figure 3. Comparison of the observations of HD 29647 by Whittet *et al.* (1981) with Mie theory results for compound core–ice mixture mantle grains: $a_c = 0.12$, $a_m = 0.132\,\mu m$, $m_c = 1.5$. Mixture 1, pure H_2O, amorphous, at 10 K; mixture 2, pure H_2O, at 10 K after annealing to 80 K; mixture 3, $H_2O/NH_3 = 3/1$ at 10 K; mixture 4, $H_2O/NH_3 = 3/1$ at 10 K after annealing to 50 K.

and in the visible respectively, expressed in magnitudes, and C_V the extinction cross-section in the visible is given by $C_V = Q_V \cdot \pi a_2^2$ and Q_V is the mean extinction efficiency in the visual. For $Q_V \simeq 1.5$ we have:

$$\frac{C_{abs}(\lambda)}{C_V} = \frac{16\pi}{\lambda}\frac{a_2^3 - a_1^3}{a_2^2}\frac{\epsilon_2}{(\epsilon_1 + 2)^2 + \epsilon_2^2} \equiv \frac{A_{abs}(\lambda)}{A_V}. \tag{3}$$

As is the case in the Rayleigh approximation for homogeneous spheres, this expression separates the effects of size from those of the optical properties of the core–mantle grains, so that changes in one of these parameters can be studied independently of the other. Using $a_1 = 0.12$, $a_2 = 0.132\,\mu m$, $m_2 = 1.29 - i\,0.324$ and $\lambda^{-1} = 0.328\,\mu m^{-1}$ at the peak of the absorption coefficient for the unannealed mixture $H_2O : NH_3 = 3 : 1$, representing 75 per cent H_2O, one gets $A_{abs} \sim 0^m.12$ for $A_V = 3^m.5$. This value of $A_{abs}(\lambda)$ is a bit larger than to be expected because the true mantle is not likely to contain more than 60 per cent H_2O, but this value already compares very favourably with the approximate value of $A_{abs} \sim 0^m.1$ deduced by Goebel from his observations. One derives from Fig. 8 in Greenberg *et al.* (1983) that for a mixture representing 60 per cent H_2O ice, $m''_{60\,per\,cent} \simeq 0.75 \times m''_{75\,per\,cent} \simeq 0.242$. With this number one gets $A_{abs} \simeq 0^m.09$.

It should be noted that equation (3) is a good approximation, valid to within 10 per cent so long as ϵ_2 is not too large, say $\epsilon_2 \lesssim 1$, and so long as there is no core absorption.

3 Band shape calculations

In Fig. 3 we show a comparison of our calculated results, using the Mie theory for core–mantle particles for various mixtures in the mantle, with the observations by Whittet *et al.* Note that this again is approximate for several reasons, one of which is the fact that we have used spheres rather than elongated particles, whereas polarization has been observed in the visual (McMillan & Perry 1981). For a discussion of shape effects see section 7 in Greenberg *et al.* (1983). Furthermore, we calculated the extinction efficiencies $Q_{ext}(\lambda)$ using single sizes instead of a size distribution. However, in view of the poor quality of the data shown in Fig. 1, this added detail would not make any difference.
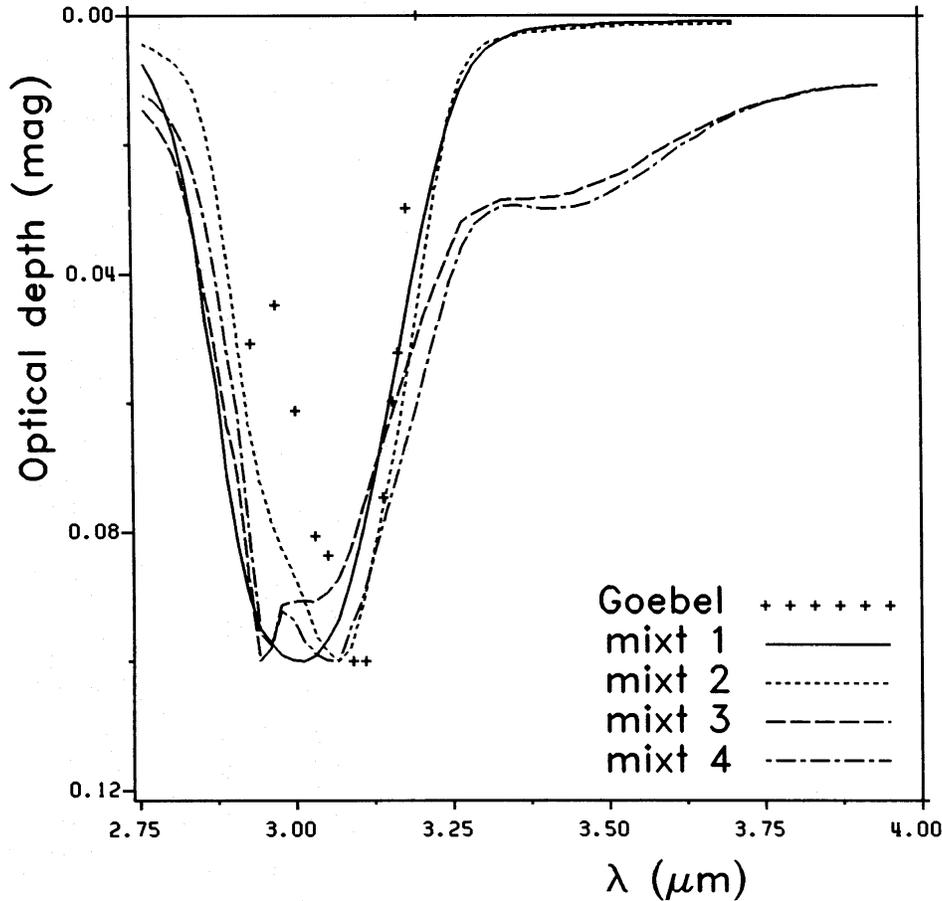
Figure 4. Comparison of the observations of HD 29647 by Goebel (1983) with Mie theory results for compound core–ice mantle grains: $a_c = 0.12$, $a_m = 0.132 \,\mu$m, $m_c = 1.5$. The mixtures are the same as in Fig. 3.

From the calculated efficiencies we derived $E(\lambda-V)/E(B-V)$ using the expression:

$$\frac{E(\lambda-V)}{E(B-V)} = \left[\frac{Q_{ext}(\lambda)}{Q_V} - 1\right] \times R, \tag{4}$$

in which Q_V is the value for the extinction efficiency in the visual, estimated to be 1.5, and $R = 3.45$. The only effect of using a lower value for R than that given by Whittet *et al.* is to raise the figure a little bit and give a better match to the observed values. The shape of the calculated ice band is not affected.

In the calculations we used as size parameters $a_1 = 0.12$ and $a_2 = 0.132 \,\mu$m; for the core we used an index of refraction $m_1 = 1.5$, for the mantle we used our laboratory measured values of four different mixtures, i.e. mixture 1, H_2O (amorphous, at 10 K); mixture 2, the same, but after annealing to 80 K; mixture 3, $H_2O : NH_3 = 3 : 1$ at 10 K; and mixture 4, the same as mixture 3 but after annealing to 50 K. It is immediately seen that the strengths of the calculated bands are of the right order. Mixtures 1, 3 and 4 show a broad absorption which is even somewhat too weak. However, by using an extra absorption in the core, say $m'' \simeq 0.05$, or bigger mantles, $a_2 \simeq 0.14 \,\mu$m, the strength will increase. Our conclusion has to be that the observations of Whittet *et al.* cannot disprove the presence of an ice band towards HD 29647. The profile of mixture 2 (pure, annealed ice) looks too sharp but is more consistent with Goebel's (1983) data as will be shown in Fig. 4.
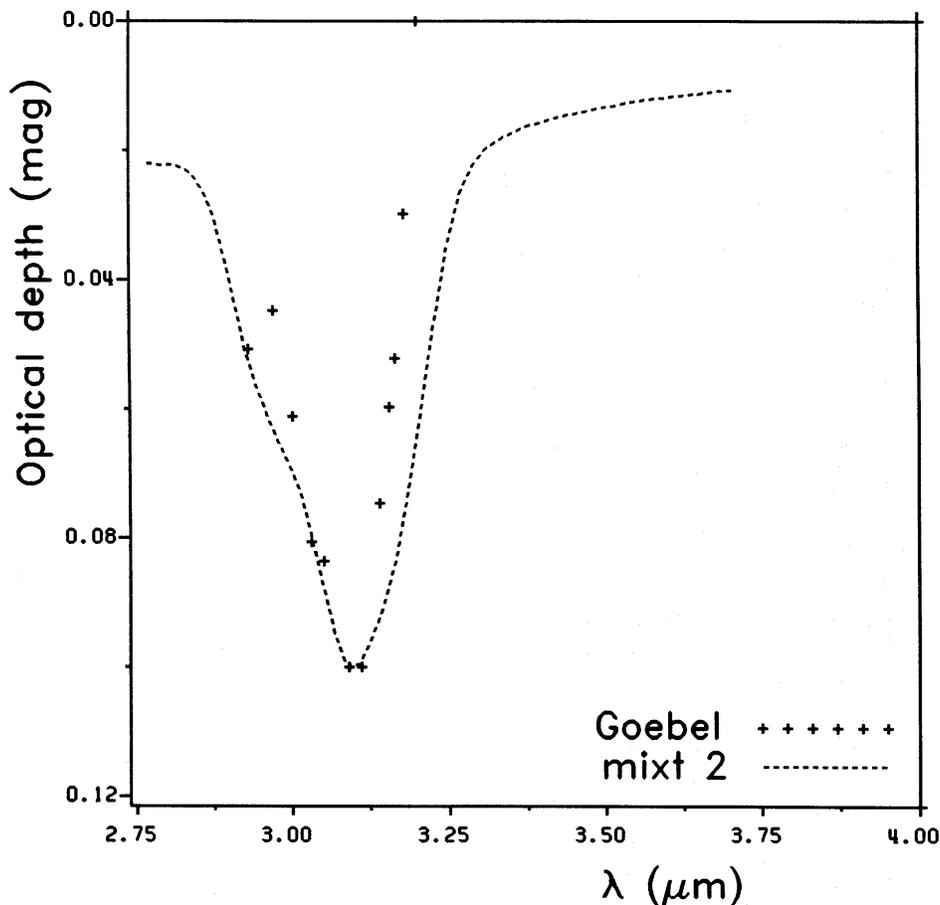
Figure 5. Comparison of the observations of HD 29647 by Goebel (1983) with infinite cylinder calculations for compound core–ice mantle grains: $a_c = 0.12$, $a_m = 0.132\,\mu m$, $m_c = 1.5$. For the ice band we used mixture 2: pure H_2O, at 10 K after annealing to 80 K.

For comparison with the calculation presented in the paper of Whittet *et al.* we have added in Fig. 1 our calculations using their parameters: $a_1 = 0.20$, $a_2 = 0.22\,\mu m$ (i.e. $x = a_2/a_1 = 1.10$), $m_1 = 1.60 - i\,0.001$ and using the optical constants for ice as obtained by Léger *et al.* (1983). It seems that there has unfortunately been a computational error in their calculations, resulting in an exaggerated enhancement of band strength and therefore misleading them to their conclusion that there is no ice towards HD 29647. Finally, we remark that their core radius of $0.2\,\mu m$ implies a basic diffuse cloud grain size which gives an anomalously large value of R.

To test our model against the observations by Goebel (1983) we have plotted in Fig. 4 the extinction efficiencies Q_{ext} from the above calculations normalized to fit Goebel's data as regards the strength of the absorption band. Included in this figure are his observations. From the sharpness of the observed band, it is clear that the best comparison can be obtained by using pure, annealed H_2O ice (mixture 2); however, the wavelength of maximum absorption is too small (3.05 instead of 3.11 μm).

As we have shown in Greenberg *et al.* (1983) the peak position shifts towards longer wavelength with increasing elongation. Now, using infinite cylinders instead of spheres we calculate a maximum at $\lambda = 3.105\,\mu m$. This is shown in Fig. 5.

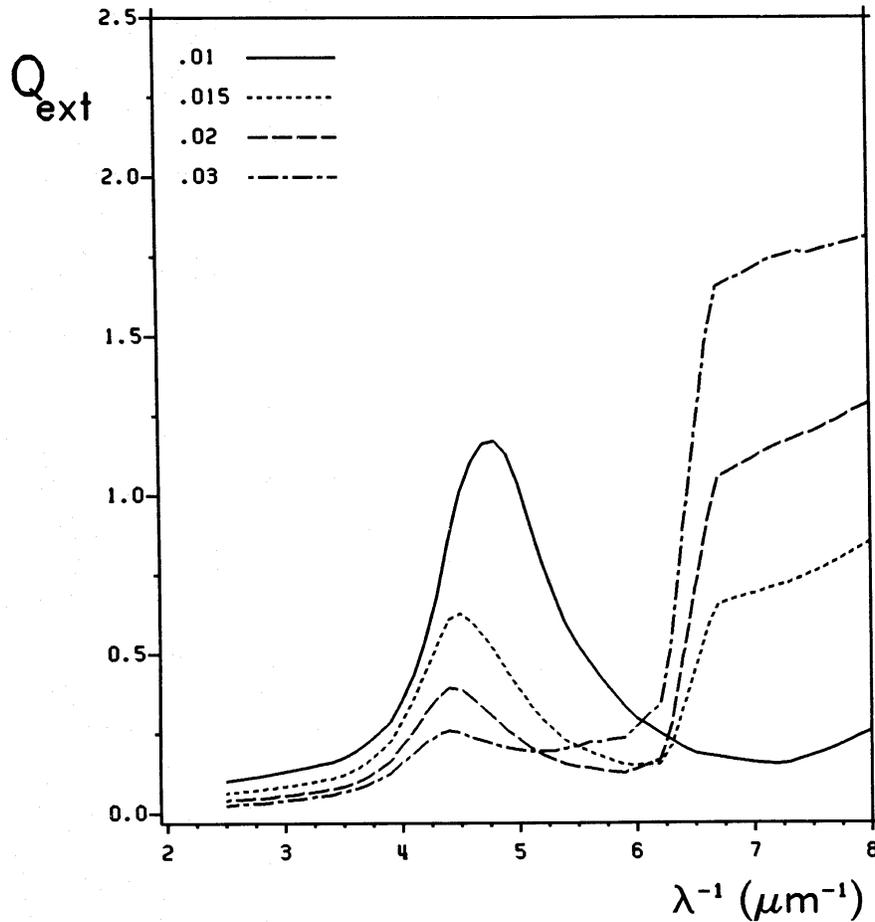Summing up, we conclude that the data are clearly consistent with the prediction of a

Figure 6. Extinction efficiencies in the ultraviolet for a graphite core with various H_2O ice mantle thicknesses. Graphite radius $a_c = 0.01$ μm; mantle radii $a_m = 0.01, 0.015, 0.02, 0.03$ μm.

core/mantle/mantle grain but that for this particular star HD 29647 the ice band is too weak to provide an accurate measure of the mixture.

4 The absence of the 2200 Å hump

To test the hypothesis that ice mantles covering the graphite grains are responsible for the absence of the 2200 Å hump — irrespective of the problems involved in accreting mantles on such small grains (Greenberg & Hong 1974; Purcell 1976; Allen & Robinson 1975; Greenberg 1979) — we did Mie theory calculations on appropriate graphite core—ice mantle grains. It is not reasonable to use mantle thicknesses greater than those derived for the core—mantle grains responsible for the 3μm ice absorption, since in uninhibited accretion processes the thickness increase is independent of the size of the particle.

The dielectric constant of graphite in the basal plane, $\epsilon_\perp$, is given by Taft & Philipp (1965); values of $\epsilon_\parallel$ are measured by Tosatti & Bassani (1970). For the ice mantles we used the values as given in the compilation of Greenberg (1968).

In Fig. 6 are plotted the extinction cross-sections $\bar{C}_{ext}$ for the graphite core—ice mantle grains for several sizes: $a_1 = 0.01 \mu$m, $a_2 = 0.01$ (no mantle), 0.015, 0.02 and 0.03 μm respectively, where $\bar{C}_{ext}$ is defined as the weighted mean of the extinction cross-sections calculated using $\epsilon_\perp$ or $\epsilon_\parallel$ for graphite; namely: $\bar{C}_{ext} = (2\ C_{ext}^\perp + C_{ext}^\parallel)/3$, as is the case if the
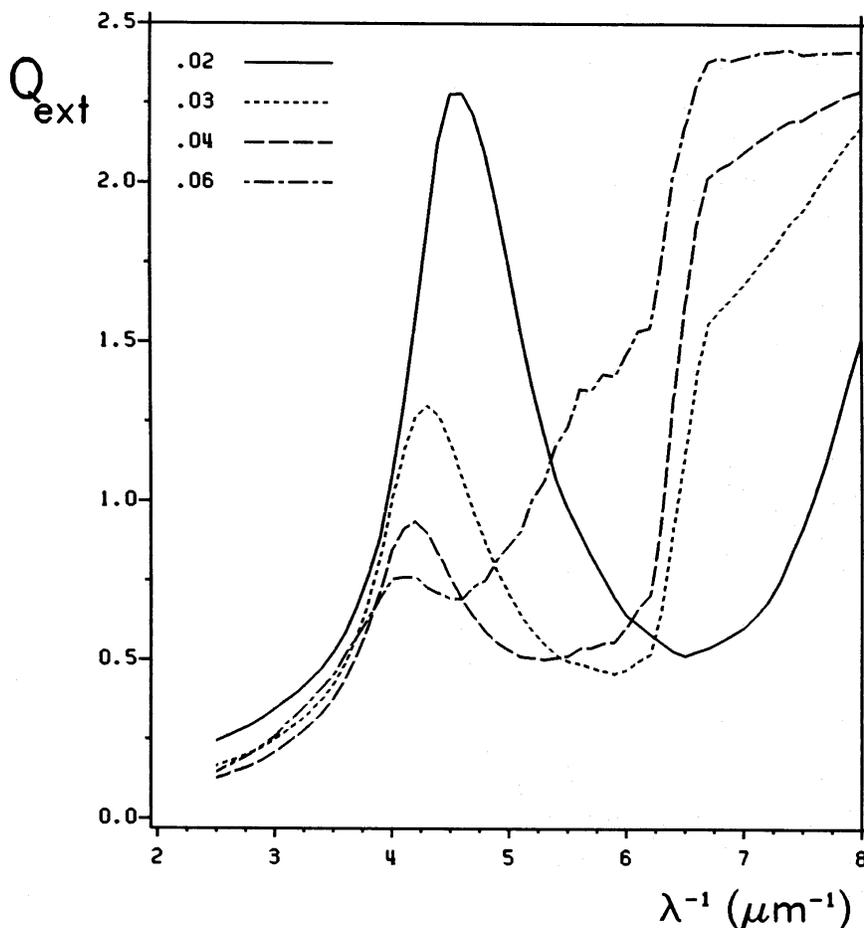
Figure 7. Same as Fig. 6 but with larger grain sizes. Graphite radius a_c = 0.02 μm; mantle radii a_m = 0.02, 0.03, 0.04, 0.06 μm.

particles are randomly orientated and small compared to the wavelength. For larger particles this averaging is not correct (Wang & Greenberg, 1976).

It is to be seen that there is a shift in the wavelength of the maximum of the peak absorption from 2100 Å (4.75 μm^{-1}) for the bare graphite particles towards about 2175 Å (4.6 μm^{-1}) for the core—mantle grains as noted earlier by Gilra (1972). However, it is impossible to remove the absorption feature unless one were to use entirely unrealistic mantle sizes.

This is also evident in Fig. 7, where we used larger grain sizes, i.e. a_1 = 0.02 μm and a_2 = 0.02 (no mantle), 0.03, 0.04 and 0.06 μm. In this case the maximum shifts from 4.55 μm^{-1} towards about 4.3 μm^{-1}. Even in the case of the larger graphite core — ice mantle grains the rapid rise in the far-ultraviolet extinction cannot obscure the 2200 Å hump.

From these results we conclude that towards HD 29647 it is impossible to eliminate the 2200 Å hump by covering the grains responsible for this feature with ice mantles. This conclusion holds no matter what the carrier is of the 2200 Å hump since the effect of a mantle is qualitatively independent of the core.

5 Conclusions

We have shown that the grains towards HD 29647 have an ice band whose shape and depth as predicted by theoretical calculations are consistent with observations. Furthermore, we have shown that the absence of the 2200 Å extinction hump cannot be attributed to

accreted mantles on graphite grains whose thicknesses are consistent with those required for the ice band strength. We conclude therefore that the absence of the 2200 Å hump implies in fact a substantial depletion of the 2200 Å hump particles.

Acknowledgment

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