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# INFRARED EXTINCTION CROSS SECTIONS OF SILICATE GRAINS

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Extinction cross sections for plagioclase and pyroxene silicate particles have been calculated for frequencies between 10 and 1400 $cm^{-1}$. Results are compared to infrared observations of grains.

*Key words:* extinction — grains — silicates — infrared

## I. Introduction

Much progress in the understanding of the grains has come through observations at wavelengths shorter than 25 $\mu$, and it is expected that the wavelength region between 25 $\mu$ and 1 mm will also provide information pertaining to the grains. Indeed, significant far infrared emission has been observed and attributed to emission by hot grains in H II regions (Hoffmann, Frederick, and Emery 1971*a*; Harper and Low 1971; Soifer, Pipher, and Houck 1972), the galactic center (Hoffmann, Frederick, and Emery 1971*b*; Gezari, Joyce, and Simon 1973), and possibly extragalactic objects (Aumann and Low 1970). Because of the availability of this new information and the probable imminence of a great deal more, we are investigating how it can be applied to elucidating the nature of the grains.

There is now fairly strong evidence for three different grain types. Ultraviolet observations indicate graphite grains (Gilra 1971) while features near 10 $\mu$ and 20 $\mu$ in the spectra of circumstellar shells and interstellar absorption indicate that some grains are silicates (cf. review by Woolf 1973). Recent observations point to the existence of water ice in dark clouds (Gillett and Forrest 1973). This picture may become more complex in the future; but in whatever way it evolves, the existence of large amounts of silicate material now appears to be established. Thus it seems appropriate that the far infrared extinction properties of silicate grains, for which the requisite optical constants are available, be investigated. Knowledge of these properties may provide new insights into the problem of chemical identifications of the grains and into the physical processes responsible for infrared emission and extinction.

## II. Silicate Solid Properties

Astronomical studies of the grains have been hampered by the lack of data describing optical properties of possible grain materials. Gaustad (1963) combined transmission measurements of several minerals to estimate an extinction curve. However, this kind of data cannot include particle scattering or resonance effects (Martin 1971). For accurate extinction cross sections, knowledge of the dielectric constant, $\epsilon = \epsilon_1 - i\epsilon_2$, or equivalently, the complex index of refraction, is required. Knacke (1968) calculated extinction cross sections for quartz and silica grains between 1 $\mu$ and 14 $\mu$. While this was an accurate calculation, it was an oversimplified model which could only show that a strong band existed near 10 $\mu$ which could be used to identify silicates.

Following a theoretical prediction by Gilman (1969), Woolf and Ney (1969) argued strongly for a mineral composition such as olivine or pyroxene. Such minerals provide a fair fit to the emission spectra of a number of stars, of the Orion H II region (Stein and Gillett 1969), and of comets (Maas, Ney, and Woolf 1970). The condensation of a cooling gas has also been investigated by Larimer (1967) and by Larimer and Anders (1967) in an investigation of fractionation of meteorites. An experimental study by Meyer (1971) demonstrated fractionation and condensation in a laboratory environment approximating conditions in circumstellar clouds. These investigations show that a number of different silicates

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will condense with temperature-dependent fractionation of elements such as Mg, Si, Fe, Ca, and Al. Thus one can conclude that observation, experiment, and theory indicate that silicate condensates of varying relative abundances will form in the circumstellar environments of both young and old stars. The material is not in the form of pure silicas but most likely is similar to meteoritic material. In astronomical applications the detailed composition of the grains will have to be determined by remote sensing methods so that intercomparison of optical properties of different silicates is essential.

Recently, dielectric constants as a function of frequency (10–1600 $\text{cm}^{-1}$) for a number of silicate minerals have been measured by Perry et al. (1972). The silicates are *lunar* material and the data are, to our knowledge, the most complete for silicates. Lunar rocks are more rich in plagioclase ($(\text{Ca, Na})(\text{Al, Si})_4\text{O}_8$) and pyroxene ($(\text{Mg, Fe})_2\text{Si}_2\text{O}_6$) minerals than meteorites in which the most abundant mineral is olivine ($(\text{Mg, Fe})_2\text{Si O}_4$). Since meteorites and circumstellar grains may be formed in similar processes, it would also be interesting to study olivine minerals for comparison to grain spectra. Unfortunately, we have not found infrared dielectric properties of olivines in the literature.

In Table I we reproduce the mineral abundances of selected samples from Perry et al. In the last column, labeled "laboratory basalt," we list the abundances of the basalt used by Meyer (1971) as a target in his condensation experiments, to show the similarity to the lunar material. In Meyer's experiment, at temperatures below 573° K, the composition of condensates was within a few percent of the values of the laboratory basalt except for MgO which varied between 5% and 7% in different runs. Fractionation occured at temperatures between 573° K and 1273° K with compounds of Mg, Si, and Fe having lower sticking probabilities than Ca or Al.

## III. Extinction Cross Sections

Extinction factors $Q$ (cross section for extinction divided by geometrical cross section) have been calculated for a number of silicates from a formula given by van de Hulst (1957). When the ratio of particle diameter to wavelength is small, the extinction factor can be approximated by the expansion

$$Q = -4\chi \,\text{Im}\left(\frac{\epsilon - 1}{\epsilon + 2}\right) - \frac{4}{15}\chi^3 \,\text{Im} \cdot \left[\left(\frac{\epsilon - 1}{\epsilon + 2}\right)^2 \left(\frac{\epsilon^2 + 27\epsilon + 38}{2\epsilon + 3}\right)\right] + \frac{8\chi^4}{3}\,\text{Re}\left(\frac{\epsilon - 1}{\epsilon + 2}\right)^2 ,$$

where $\chi = 2\pi a\nu$, $a$ is particle radius, and $\nu$ is the wavenumber. The first term is the classical Rayleigh absorption cross section, and is dominant for small $\chi$ which is the case in the infrared for the particles considered in this paper.

Grains of differing compositions are found to have different mean radii when a fit is forced to the interstellar extinction curve, but the total range in grain sizes for all suggested models is only about 0.02 $\mu$ to 0.5 $\mu$. Knacke (1968) found that the visible extinction curve could be fitted tolerably well with extinction by silica grains of radius $a = 0.2\ \mu$. Consequently, 0.2 $\mu$ may be a representative size and is used in the calculations in this paper.

TABLE I

MAJOR OXIDE ABUNDANCE, PERCENT

| Oxide | 14310 | 14321 | 10058 | 12009 | 12065 | Laboratory Basalt |
|---|---|---|---|---|---|---|
| $\text{SiO}_2$ | 50 | 50–48 | 41 | 41 | 39 | 49 |
| $\text{Al}_2\text{O}_3$ | 20 | 18–14 | 11 | 11 | 12 | 13 |
| MgO | 8 | 12–11 | 6 | 12.5 | 9 | 6 |
| FeO | 8 | 13–9 | 17 | 20 | 22 | 11 |
| CaO | 11 | 9–8 | 12 | 10 | 12 | 11 |
| $\text{TiO}_2$ | 1 | 2–1 | 11 | 3 | 4 | |
| (Fe/Ti) oxide | 9 | 15–10 | 28 | 23 | 26 | |

Extinction factors for the silicates in Table I are shown in Figure 1. The term proportional to $\chi$ was found to dominate in all of the silicates in Figure 1. Consequently the calculated $Q$s can be scaled for other particle sizes until $\chi$ approaches unity.

Examination of the figures shows that extinction by silicate particles is characterized by strong absorption bands near 1000 $\mathrm{cm}^{-1}$ (10 $\mu$) and 550 $\mathrm{cm}^{-1}$ (18 $\mu$), weaker bands at frequencies less than 500 $\mathrm{cm}^{-1}$, and a rapid decrease of the cross section to lower frequencies. The absorptions at 1000 $\mathrm{cm}^{-1}$ are due to Si-O stretching modes and those near 550 $\mathrm{cm}^{-1}$ due to Si-O-Si bending modes. The other absorptions are dependent upon the cations in the material.

As observations of silicate dust become more complete, it becomes worthwhile to examine the possibilities of using the extinction properties of the grains as diagnostics for mineral abundances in the grains. These abundances are determined by the environment in which the grains formed (Larimer and Anders 1967) and, in principle, reveal the chemical and thermal history of the grains. Such a program is possible only if the absorptions are characteristic of grain constituents in a straightforward way, observable by techniques available to infrared astronomy.

The infrared bands are characterized by position, intensity, and shape. Recent efforts to relate these quantities to composition for remote sensing applications have been reported by Aronson and Emslie (1972). The dependence of band position on cation substitution in silicates follows the well-known pattern (Perry et al. 1972) that both the Si-O stretch and bending vibrations are shifted to lower frequencies with the substitution of heavy cations. The positions of maximum extinction in the bands are listed in Table II. The positions of the maxima do not quite agree with the maxima of $\epsilon_2$ because of a resonance in the equation above, also observed in quartz (Knacke 1968). Comparison of Table I and Table II shows that there may be some evidence for a systematic shift of band position with cation substitution. However, effects of inhomogeneity

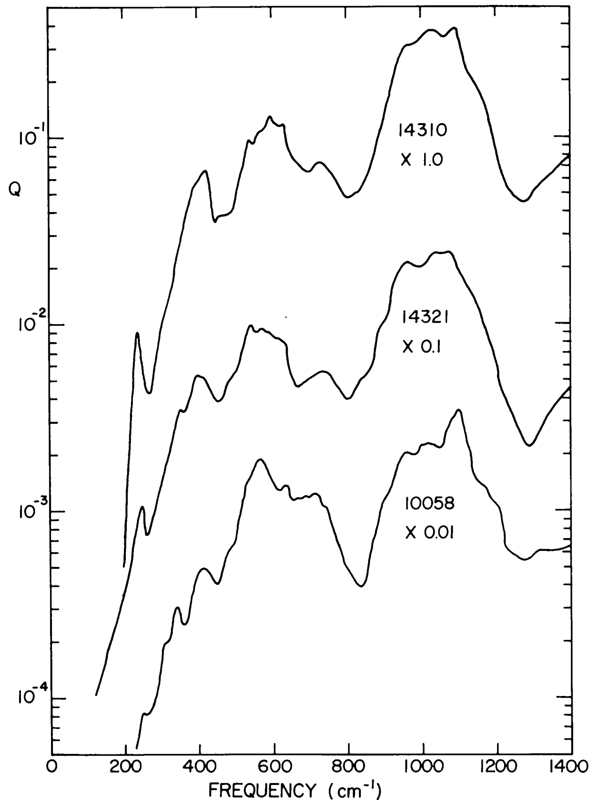

FIG. 1a — Extinction factors for silicates (see Table I).

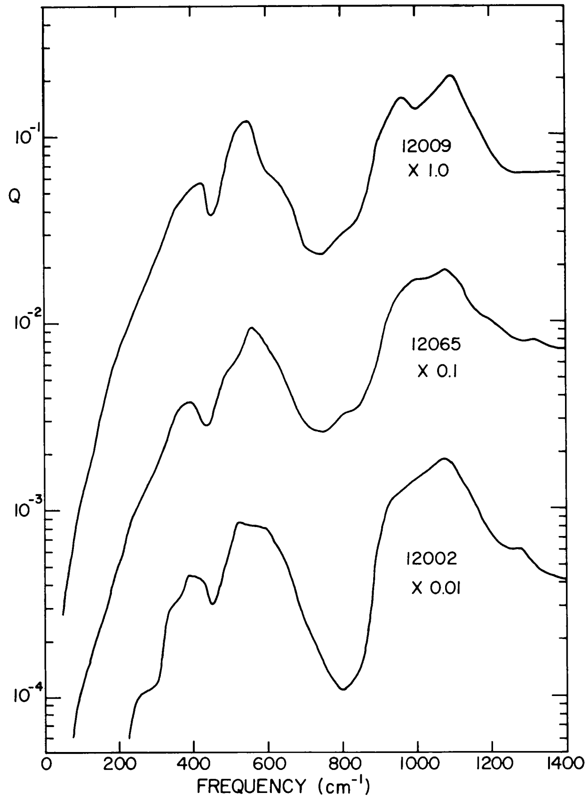

FIG. 1b — Extinction factors for silicates (see Table I).

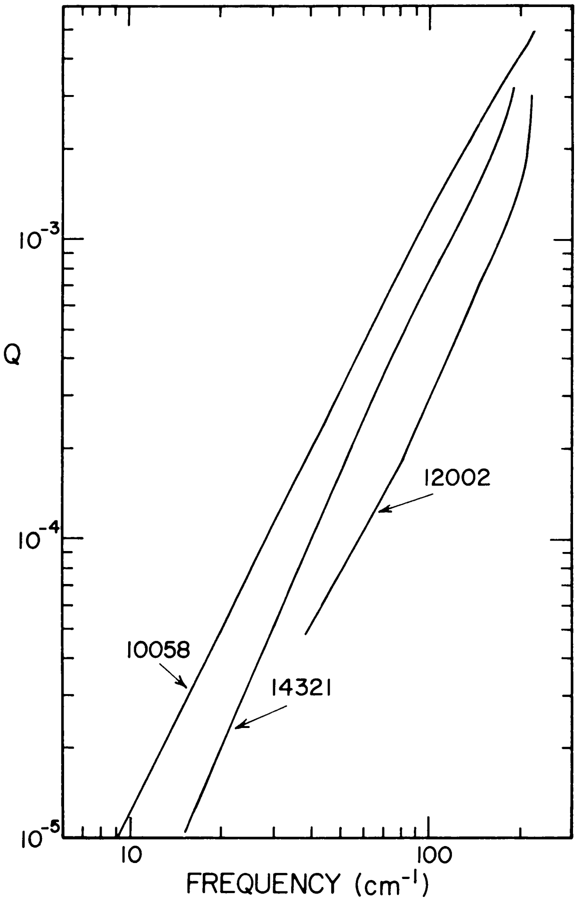

FIG. 2 — Far infrared extinction factors for silicates (see Table I).

in the samples, overlapping of bands, and small particle extinction make the interpretation of the frequency shift ambiguous.

In the last column of Table II we list the ratio of Q at the peak bending absorption (550 cm$^{-1}$) to that at the peak of the stretching absorption (1000 cm$^{-1}$). In this case there appears to be a more well-defined correlation with heavy cation content. As the amount of FeO content is increased both the $SiO_2$ and $Al_2O_3$ content decreases. Consequently the rocks change from a plagioclase character (14310) to a pyroxene character (12065), and the bending mode becomes relatively more intense. While this correlation should be checked in more samples to confirm that it is a real effect, we note that in Figure 1 of Estep, Kovach, and Karr (1971) the same correlation exists in the comparison of the spectra of a plagioclase and a pyroxene mineral. It appears that the chain structure of the pyroxene allows bending more readily than the triclinic lattice of the plagioclase. Since the relative intensity of the absorption changes by 40%, this may be a more easily observable effect in astronomical applications than the frequency shift.

A number of weak absorptions occur between 450 cm$^{-1}$ and 200 cm$^{-1}$. These have been investigated by Tarte (1963) in olivine and pyroxene materials. Tarte shows that these absorptions are much more dependent on cation properties than the stronger absorptions at high frequencies which are largely determined by the $SiO_4$ tetrahedra. The band near 240 cm$^{-1}$ is characteristic of plagioclase material (Perry et al. 1972) and its strength decreases as the minerals become more pyroxene like. The bands at these low frequencies present great difficulties for observation at the present time because of their position and weakness.

At frequencies below 200 cm$^{-1}$ the extinction factor rapidly becomes small. The submillimeter Qs are shown in Figure 3. At these frequencies the cross section approaches a power law which is close to $\nu^2$ for the minerals in this study. This far infrared behavior was discussed by Gezari et al. (1973). It follows from a simple dissipative model of the atomic oscillators in which the restoring force is proportional to velocity. The

TABLE II

POSITION AND STRENGTH OF THE ABSORPTION BANDS

| Rock | Si-O (Stretch) | Si-O-Si (Bending) | Intensity Ratio (Bending to Stretch) |
|---|---|---|---|
| 14310 | 1090 | 600 | 0.35 |
| 14321 | 1080 | 540 | 0.40 |
| 10058 | 1100 | 570 | 0.55 |
| 12009 | 1100 | 550 | 0.55 |
| 12065 | 1080 | 560 | 0.50 |

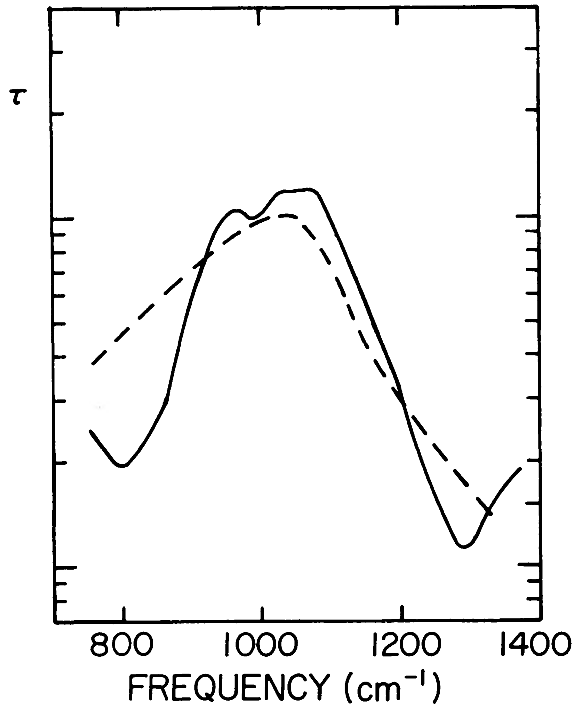

Fig. 3 — Calculated $Q$ compared to Orion emission spectrum; ——, $Q$ for rock 14321, fitted to observations at 1000 cm$^{-1}$; - - - -, observations of Orion emission (Stein and Gillett 1969).

imaginary part of the dielectric constant is then proportional to frequency, and the second power of $\nu$ comes from the factor $2\pi a\nu$ in $Q$. Hoyle and Wickramasinghe (1962) suggested this functional dependence for the extinction of graphite in the infrared.

## IV. Comparison with Observations

In Figure 3 we show $Q$ of mineral 14321 and the spectrum of grain emission in Orion (Stein and Gillett 1969). Mineral 14321 is typical of the extinction curves shown in Figure 1. The grain temperature is probably close to 300° K, so that the blackbody dependence on wavelength in the range shown in Figure 3 is small and with the assumption of small optical depth we can compare $Q$ directly with the emission spectrum. Gillett, Low, and Stein (1968) found almost identical emission spectra for a number of M stars, hence this comparison is relevant for circumstellar grains also.

The emission spectrum of the grains is similiar to that given by Woolf and Ney (1969) for olivine and the mineral mixture derived by Gaustad (1963). The agreement of our calculations and the observations is slightly better than the olivine and mineral mixtures compared by Woolf and Ney. However, at frequencies less than 1000 cm$^{-1}$ the silicate emission feature falls off considerably more sharply than the observed curve, as is also the case for olivine and somewhat less so for the mineral mixture.

This discrepancy could be either a size or a composition effect. Grains with radii greater than 1 μ are required to give anything more than a simple scaling of $Q$ with size at 1000 cm$^{-1}$. There is evidence to suggest that large grains may exist in circumstellar shells (Strom, Strom, and Yost 1971), as is expected since small grains are more readily driven away from stars by radiation pressure. However, 1 μ is larger than indicated by the results of Strom et al. A mineral constituent not included in these calculations could also give emission at 800 cm$^{-1}$. For example, silicon carbide which should be abundant in some circumstellar envelopes (Gilman 1969) has a strong absorption band near 790 cm$^{-1}$. Temperature structure in the clouds might also distort the bands, but the almost identical band shape in circumstellar clouds and in an H II region would seem to make this explanation unlikely.

The interstellar absorption feature observed in Orion by Gillett and Forrest (1973) and by Woolf and Gillett (Woolf 1973) in the galactic center is sharper than the emission in Orion. A comparison between rock 14321 and the galactic center is shown in Figure 4 where we have derived an optical depth of $\tau = 3.8$ at 1040 cm$^{-1}$. The calculated curve deviates considerably from the observations near 1200 cm$^{-1}$ but part of this may be due to the shape of the continuum. The observed absorption is also narrower than the calculated. It seems unlikely that there would be appreciable temperature narrowing of the calculated bands because of the amorphous structure of the rocks. Consequently this may be an indication that the interstellar grains may be more crystalline than the minerals investigated here. It would also be interesting to investigate other minerals such as olivine.

Soifer et al. (1972) have compared infrared emission by grains in H II regions with grain models at wavelengths between 5 μ and 100 μ. Their models are based on the assumption that

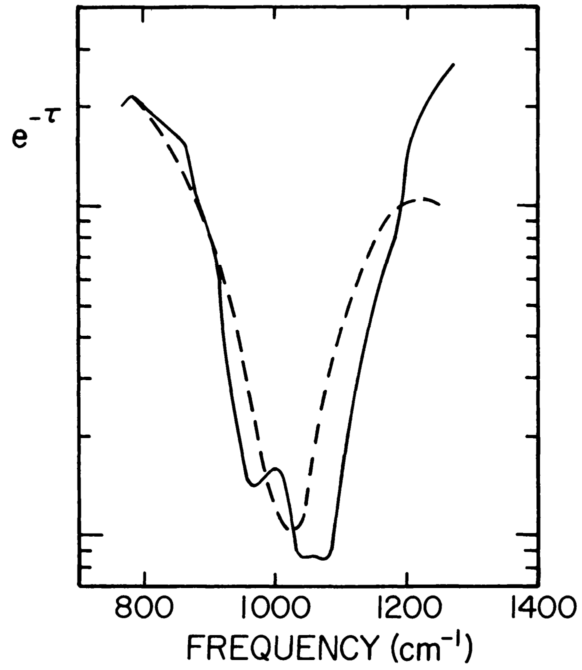

FIG. 4 — Calculated compared to observed absorption in the galactic center; ——, $e^{-\tau}$ for rock 14321 with $\tau = 3.8$ at 1040 cm$^{-1}$, fitted to observations at 800 cm$^{-1}$; - - - -, spectrum of the galactic center (Woolf 1973).

a single grain temperature throughout the H II region adequately accounts for the emission. Following an analysis similar to that of Soifer et al. we find that the total mass of the grains in an H II region is

$$\mathfrak{M} = \frac{\rho a F_\nu V}{3 Q B_\nu \Omega L}$$

where $F_\nu$ is the observed flux, and $\Omega$, $L$, and $V$ are the subtended solid angle, diameter, and volume of the nebula. By fitting the 20 $\mu$ and 100 $\mu$ fluxes of M8 given by Soifer et al. and taking an angular diameter of $5'.7$ and $L =$ 2.2 pc, we find that $T = 45°$ K and $M = 4\mathfrak{M}_\odot$ where $Q$ has been taken from Figure 1 for rock 14321.

This gives a gas to dust ratio of about 2 which is very much lower than the average value. A similar discrepancy was noted by Soifer et al. for their case with $Q$ proportional to $\nu^2$. They suggest that $Q$ proportional to $\nu$ gives a more reasonable value of M. The extinction factors calculated in this paper have an approximate $\nu^2$ dependence at wavelengths longer than 100 $\mu$ and an even stronger dependence between 20 $\mu$ and 100 $\mu$. The difficulty may lie in the assumption that the nebula has a uniform temperature. Indeed, Soifer et al. point out that their 13 $\mu$ data cannot be fitted by grains at the temperature of 51° K derived from the 20 $\mu$ and 100 $\mu$ data. Temperatures on the order of 300° K are found by Stein and Gillett (1969) in Orion and by Lempke and Low (1972) in M17. Thus it seems plausible that the ratio of the 20 $\mu$ and 100 $\mu$ fluxes are determined by both $Q$ and a temperature gradient across the nebula. The temperature distribution of the objects might be derived by systematic mapping in the far infrared.

Gezari et al. (1973) have suggested that $Q \propto \nu^2$ can account for the small ratio of radio to 350 $\mu$ emission in Sagittarii B2. This is very close to the frequency dependence found here and shown in Figure 2.

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