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Infra-red spectra of some selected minerals, rocks and products

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Forty-nine infra-red spectra (1600 to 400 cm^{-1}) of rocks, minerals and products of industrial importance have been determined. These include mica, asbestos, apatite, calcite, feldspar, kyanite, slags, fly ash, etc. They have been classified into several groups based on structural parameters and chemical groups with pertinent discussions relating to the spectral characteristics of these materials for rapid identification and characterization.

1. Introduction
In this paper, forty-nine infra-red spectra of rocks, minerals and products which are of industrial importance have been presented. The spectra of the materials were obtained during the course of several projects carried out in our laboratory. These materials were of Indian origin and collected from all over the country at different times. The spectra appear to serve the purpose of identification of rocks, and minerals within certain limitations. In general, it has been found useful to analyse a large number of unknown samples with the help of this set of spectra within a short time before detailed analysis was undertaken by other methods such as X-ray diffraction, chemical analysis, etc. An attempt has been made here to correlate the spectra of the materials with respect to similarity in structural parameters, chemical groups, etc. and as such the spectra have been classified into thirteen groups for discussion. The spectral region of interest has been limited to the range 1600 to 400 cm^{-1} and in some cases it has been extended up to 3700 cm^{-1} for studying the hydroxyl stretching bands.

2. Experimental
The spectra of these materials were taken in potassium bromide pellets using a Parkin–Elmer Model 621 spectrometer. The spectra of mica samples were taken as film pressed on KBr pellets. The instrument was calibrated using polystyrene film as standard. The pressure applied for making the KBr pellets was around 700 kg cm^{-2}. The materials were finely powdered (−325 mesh) in large quantities and representative spectra of samples were obtained in duplicate.

3. Absorption spectra
The fundamental modes of vibration which lead to absorption bands in the region under study are stretching, bending and lattice modes. The vibrational frequencies of these modes for the species under study vary considerably depending on parameters such as crystal forms, impurities in solid solution, etc. The presence of several phases of nearly similar absorption characteristics makes the study more complex, especially of rocks with variable composition.

3.1. Spectra of magnesite, calcite and aragonite
The carbonate rocks have three to four intense bands in this region (Fig. 1). The 1420 and 876 cm^{-1} region bands are more or less unaltered in the spectra of these materials. The 700 cm^{-1} band is characteristic for identification even in a mixture of these rocks because magnesite, calcite and aragonite absorb at 748, 711 and 700 cm^{-1}, respectively. The aragonite sample is not pure but mixed with calcite. Further, aragonite has an extra characteristic band at 1083 cm^{-1}.

3.1.1. Spectra of dolomite, dolomitic limestone and kankar
The spectrum of dolomite is similar to that of calcite except for the 700 cm^{-1} region band which

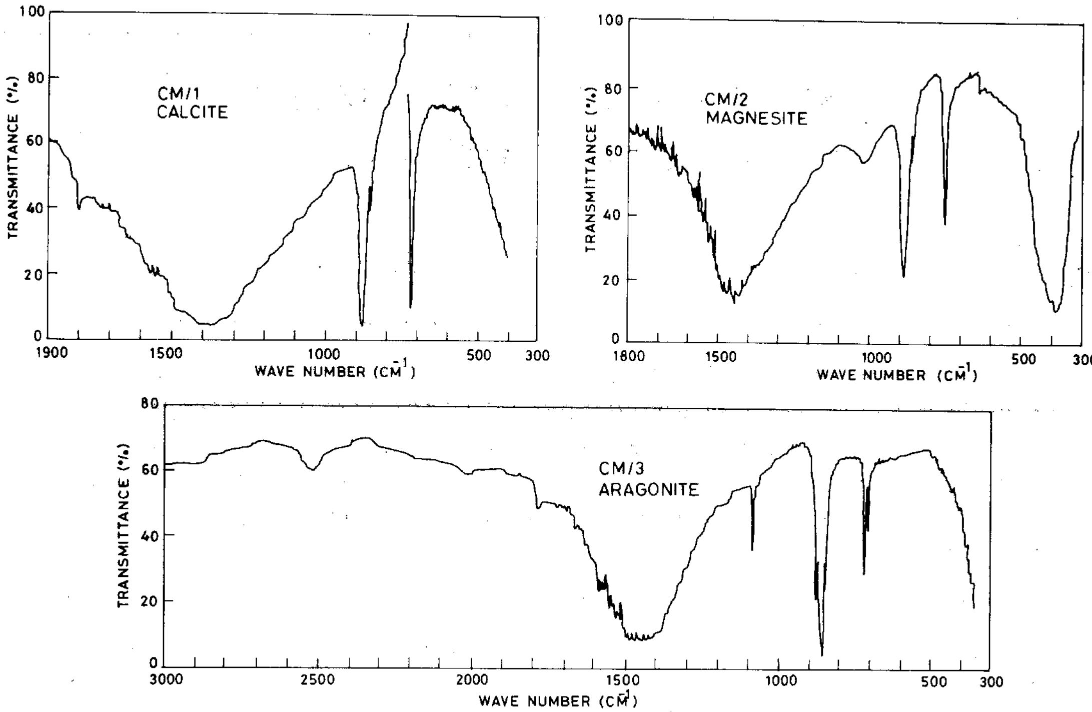
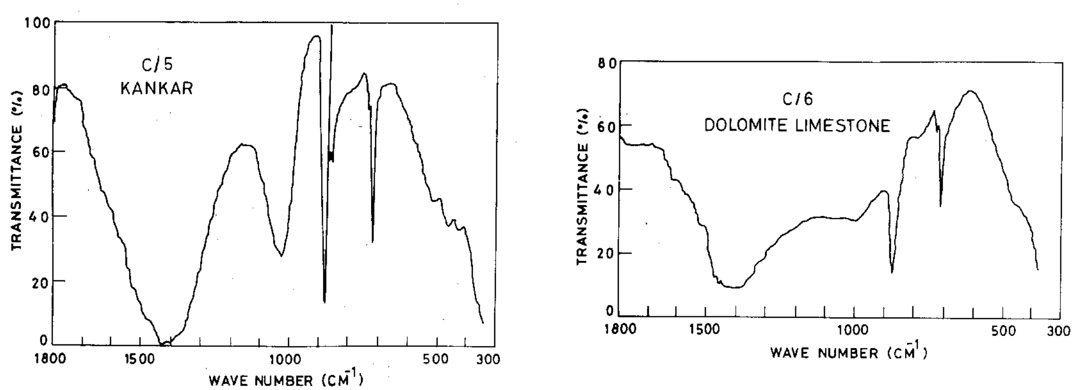


Figure 1 Spectra of magnesite, calcite and aragonite.



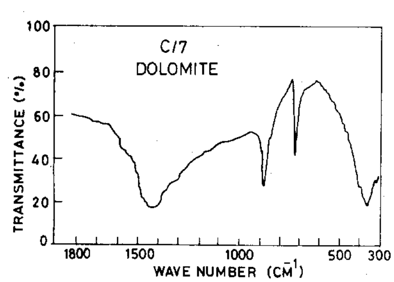


Figure 2 Spectra of dolomite, dolomitic limestone and kankar.

appears at 727 cm^{-1} in dolomite. This bands has been used for estimation of dolomite in limestone [1]. The spectrum of kankar (limestone in the form of nodules used as a raw material for the manufacture of cement in India) shows characteristic calcite and clay (1020 cm^{-1}, etc.) bands. (Fig. 2)

3.1.2. Spectra of argellaceous and silicous limestones

The spectrum of argellaceous limestone has the usual calcite bands besides the bands at 1000, 799, 510 and 462 cm^{-1}. The presence of clay is indicated. The spectrum of coral limestone indicates very little clay or silica. The spectra of silicous limestone and limestone with jasper show a high percentage of quartz as is evident from the

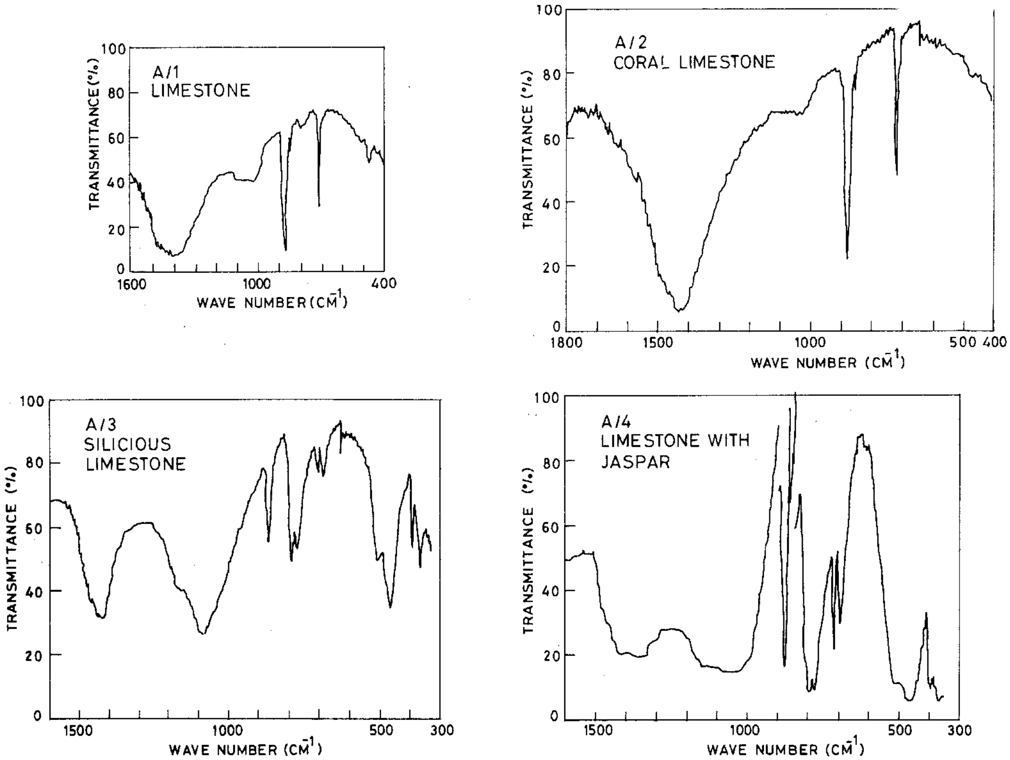


Figure 3 Spectra of argellaceous and silicious limestones.

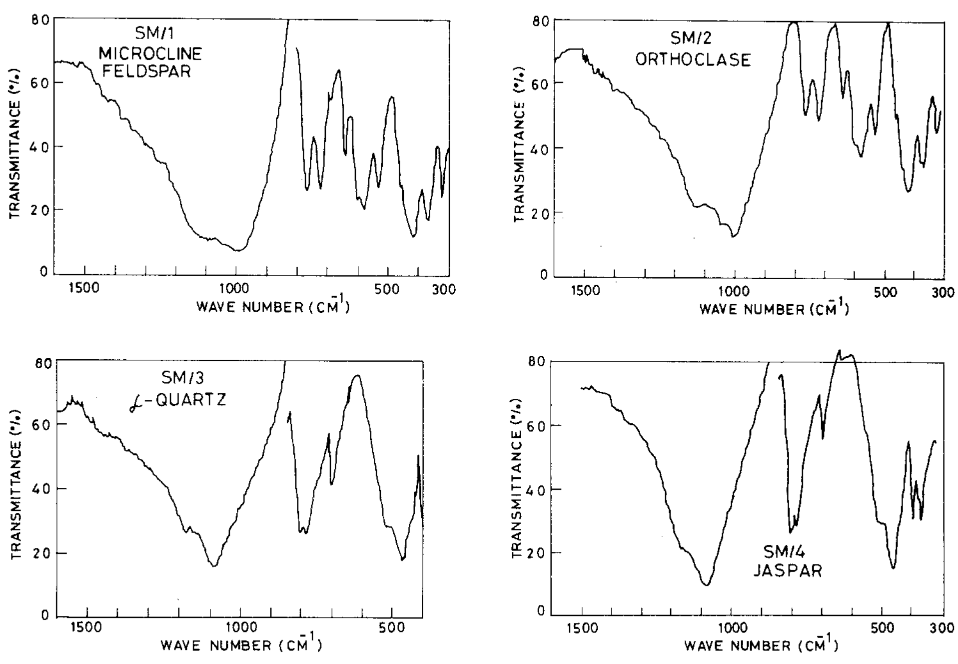


Figure 4 Spectra of feldspar, orthoclase, quartz and jaspar.

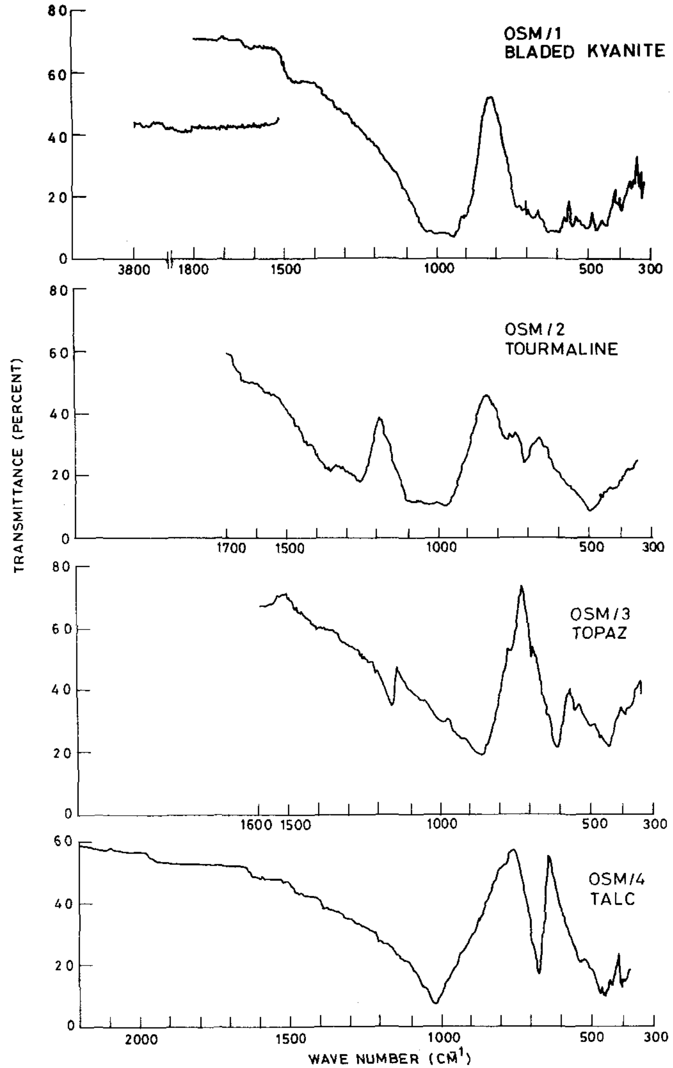


Figure 5 Spectra of tourmaline, kyanite, topaz and talc.

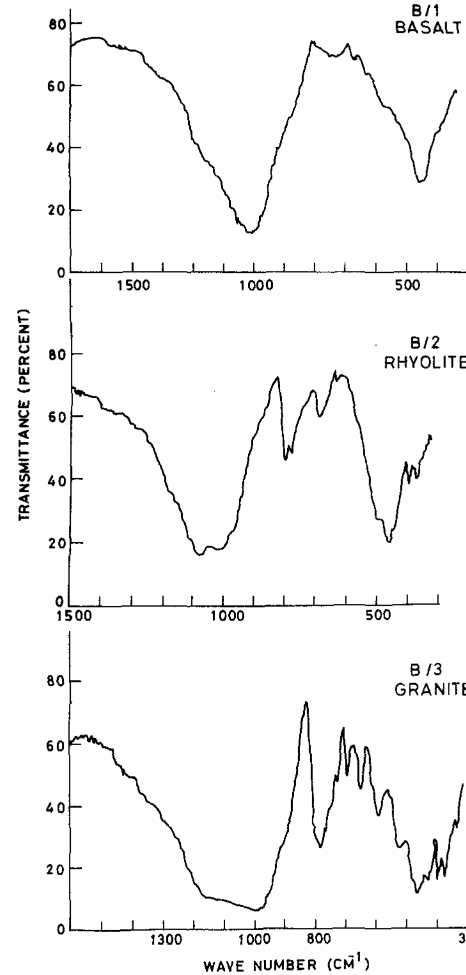


Figure 6 Spectra of rhyolite, granite and basalt.

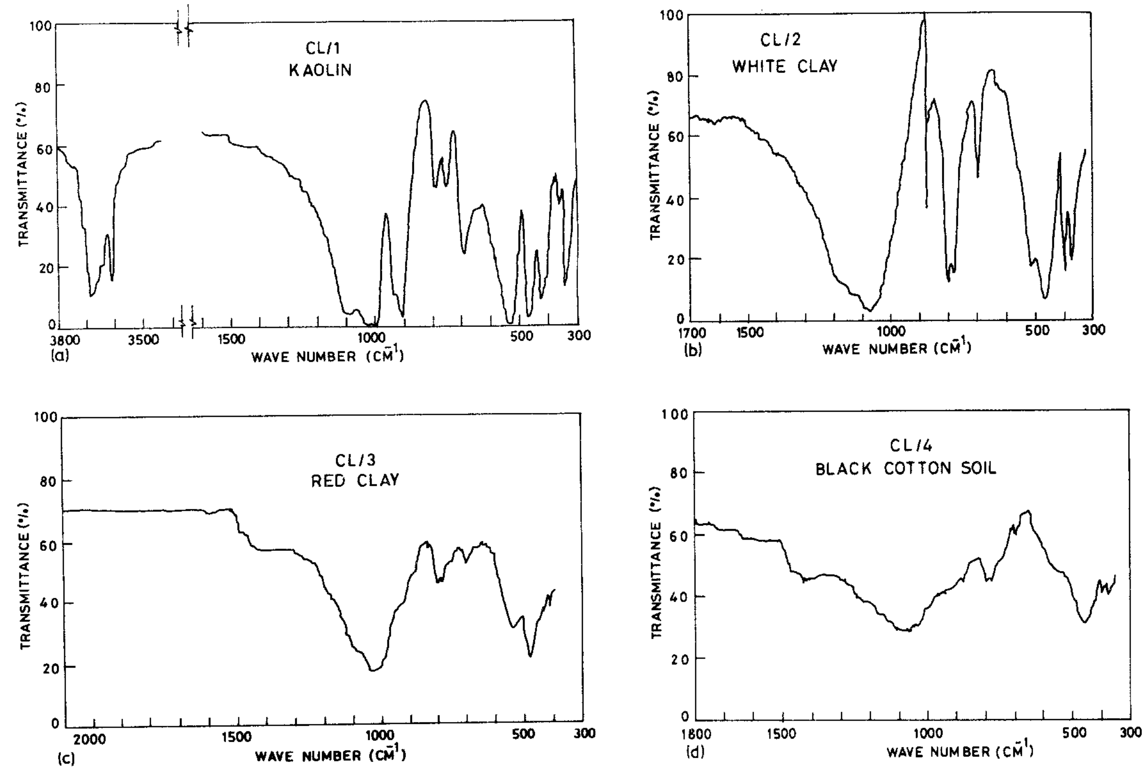


Figure 7 Spectra of kaolin and clays.

strong bands at 1165, 1090, 798, 775, 692, 515 and 465 cm^{-1}. The quartz bands in the spectrum of jaspar are broader especially at 1090 cm^{-1} indicating the crypto-crystalline nature of jaspar. (Fig. 3)

3.2. Spectra of feldspar, orthoclase, quartz and jaspar

The spectrum of orthoclase is characterized by several bands at 1138, 1050, 1010, 772, 725, 645, 603, 584, 538, 468 and 425 cm^{-1}. The spectrum of feldspar is quite similar to that of orthoclase except that the 1000 cm^{-1} band is unresolved and the main peak head in this region shifts down to 980 cm^{-1} with slight shifting of other bands. The spectra of α-quartz and jaspar are almost identical except some differences in band positions; for example, jaspar has a band at 1165 cm^{-1} while α-quartz has this band at 1175 cm^{-1}. (Fig. 4)

3.3. Spectra of tourmaline, kyanite, topaz and talc

The spectra of topaz and talc consist of few absorption bands. The spectrum of topaz has a characteristic medium intensity band at 1162 cm^{-1}, a shoulder at 1000 cm^{-1} and the main band head in this region at 865 cm^{-1}, while the spectrum of talc has a weak shoulder at 1050 cm^{-1} and the main band head is at 1015 cm^{-1}. The other characteristic bands are at 670 and 615 cm^{-1}. The hydroxyl stretching band appears at 3636 cm^{-1} in the spectrum of topaz. Kyanite, being a nesosilicate (same as topaz) has a complex spectrum below 750 cm^{-1} unlike that of topaz. The spectrum of tourmaline (cyclosilicate) has a characteristic doublet at 1300 and 1000 cm^{-1}. The spectrum has some similarity with that of kaolinite below 800 cm^{-1}. (Fig. 5)

3.4. Spectra of rhyolite, granite and basalt

The spectrum of granite indicates the presence of quartz (sharp band at 697 cm^{-1}) and orthoclase (at 650 cm^{-1}). The other regions are overlapped The spectrum of basalt is simple since the principal constituents, albite and anorthite have Si_3O_8 units and overlap in the same region. The spectrum of rhyolite shows the presence of quartz (bands at 800 and 780 cm^{-1}), but the presence of feldspar cannot be detected in its spectrum because of the amorphous nature of feldspar. (Fig. 6)

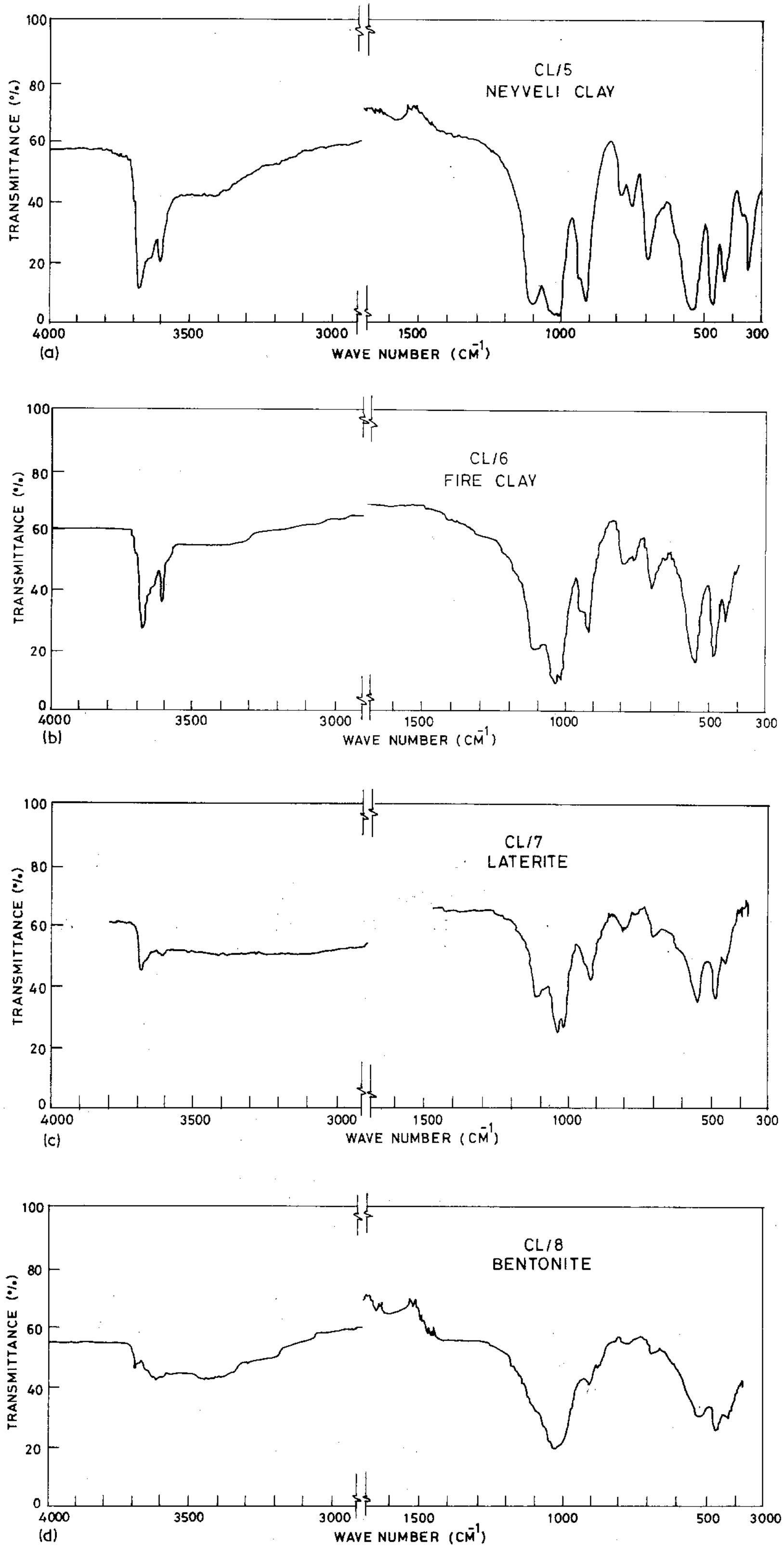


Figure 8 Spectra of bentonite, laterite, and other clays.

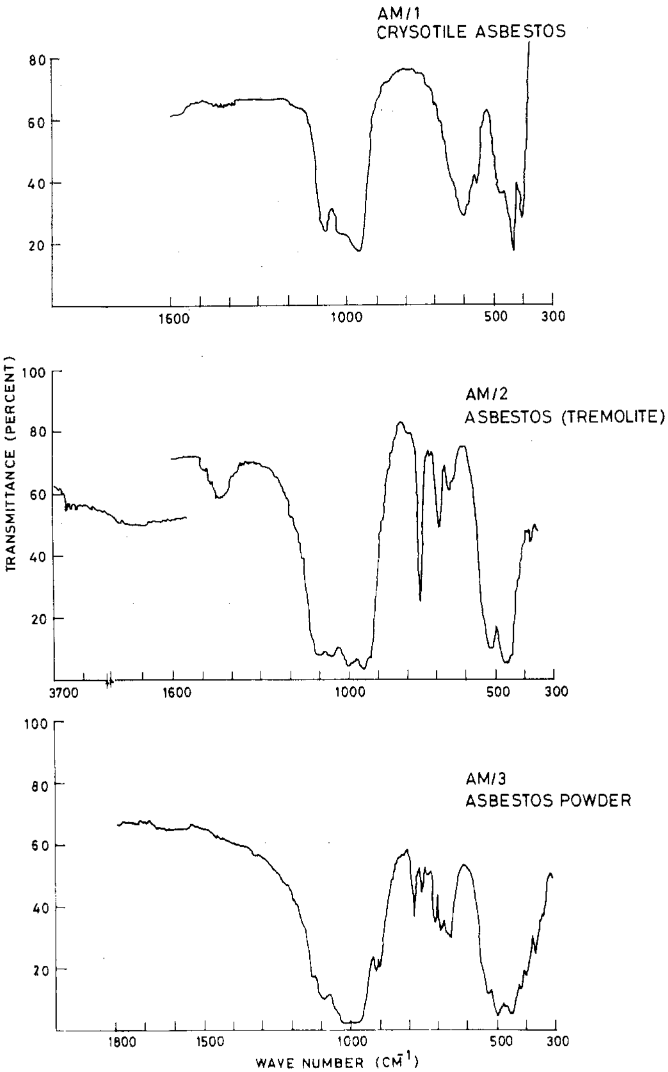


Figure 9 Spectra of chrysotile, tremolite and asbestos.

3.5. Spectra of kaolin, red clay, black cotton soil and white clay

The spectrum of kaolin is characterized by bands in the 3600 cm^{-1} region (hydroxyl stretching); at 1150 to 960 cm^{-1} (SiO stretching region) and below 960 cm^{-1} (bending and lattice modes). The spectrum of white clay shows a broad and unresolved band in the Si–O stretching region and the presence of quartz (800 and 695 cm^{-1}) is indicated. The Si–O stretching band appears at 1025 cm^{-1} (red clay) and at 1070 cm^{-1} (white clay). The spectrum of black cotton soil is diffuse and the soil sample is very poorly crystalline. Neyveli clay and fire clay are principally kaolinitic. The spectrum of bentonite indicates the presence of montmorillonite mineral, for example, bands at 1102, 1030, 915, 521 and 467 cm^{-1} [2]. The spectrum of laterite closely resembles those of kaolinite, goethite, gibbsite, etc. which are the constituents of laterite and have bands in the same region [3]. (Fig. 7 and 8)

3.6. Spectra of chrysotile, tremolite and asbestos

The spectra of chrysotile and tremolite are different. The former consists of Si_2O_5 double-layers while the latter has Si_4O_{11} units in the structure. The 1000 cm^{-1} Si–O stretching region has multiple bands in the spectrum of tremolite. The presence of carbonate in tremolite is shown by the weak band at 1400 cm^{-1}. The spectrum of asbestos (poor) shows some bands (800 to 600 cm^{-1}) common to tremolite, but the bands near 900 cm^{-1} are not present in chrysotile or tremolite. (Fig. 9)

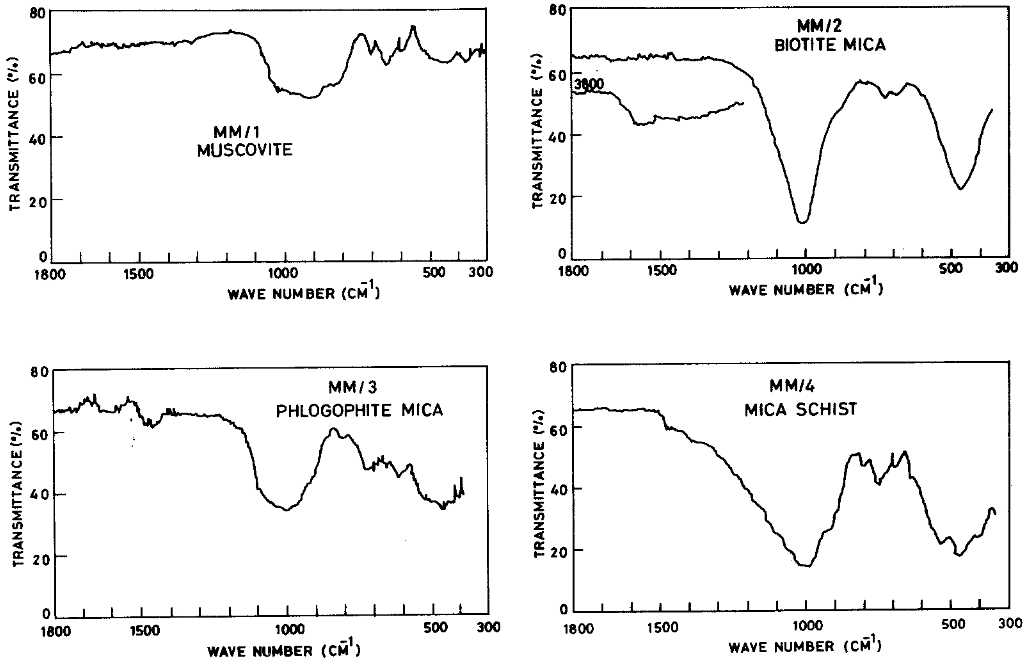


Figure 10 Spectra of biotite, muscovite mica, schist, and phlogophite.

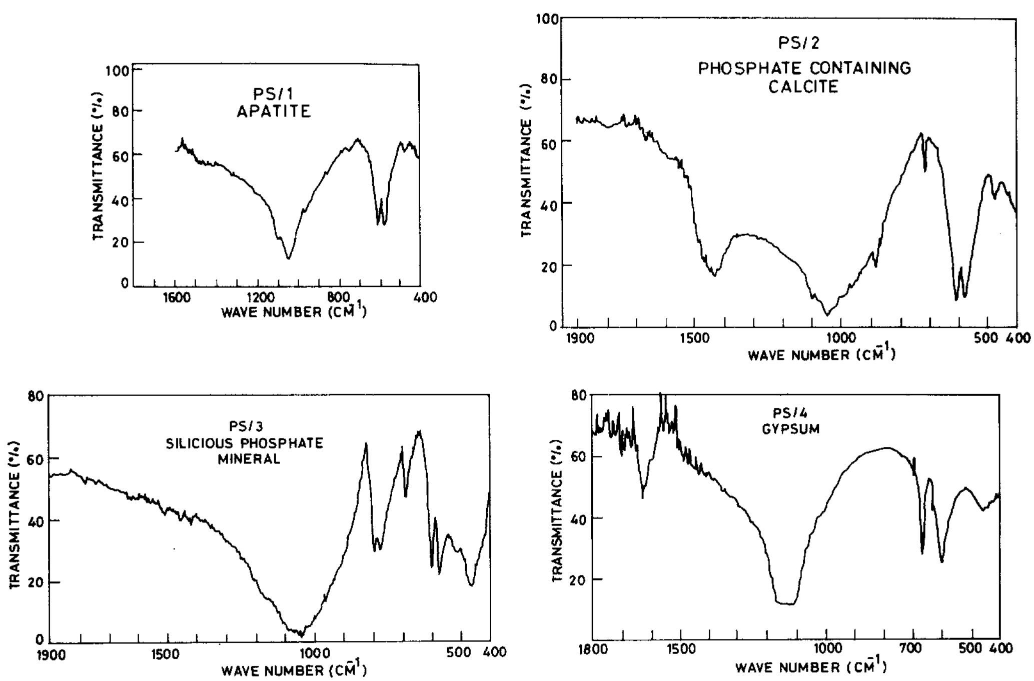


Figure 11 Spectra of apatites and gypsum.

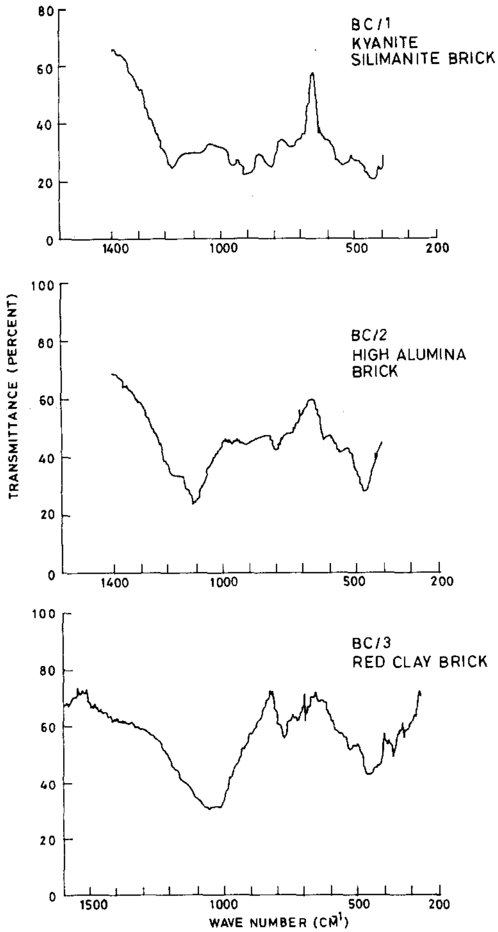


Figure 12 Spectra of bricks.

3.7. Spectra of biotite, moscovite, mica schist and phlogophite mica

The mica group belongs to phyllosilicate. Each SiO_4 unit is linked to three other SiO_4 groups similar to that in talc. The spectrum of biotite mica is characterized by strong bands at 1018 and 465 cm^{-1} and two weak bands at 728 and 685 cm^{-1}. The spectra of mica schist and muscovite are similar; the band in the 1000 cm^{-1} region is fairly broad. The spectrum of phlogophite is different to moscovite in the 800 to 600 cm^{-1} region. (Fig. 10)

3.8. Spectra of apatite, phosphatic rocks and gypsum

The spectrum of apatite rock is characterized by strong bands at 1040, 610 and 570 cm^{-1}, while that of gypsum is identified by the bands at 1140, 668 and 602 cm^{-1}. The spectrum (PS/2, Fig. 11) indicates the presence of apatite and calcite (1430, 876 and 711 cm^{-1} bands) in this sample. Similarly, the spectrum (PS/3, Fig. 11) of the apatite sample, indicates the presence of quartz (799, 780, 690 and 462 cm^{-1}).

3.9. Spectra of red clay, high alumina, and kyanite–silimanite brick samples

The spectrum of the red clay brick sample does not indicate a large quantity of quartz. The general broad spectral feature (1030 and 460 cm^{-1}) in-

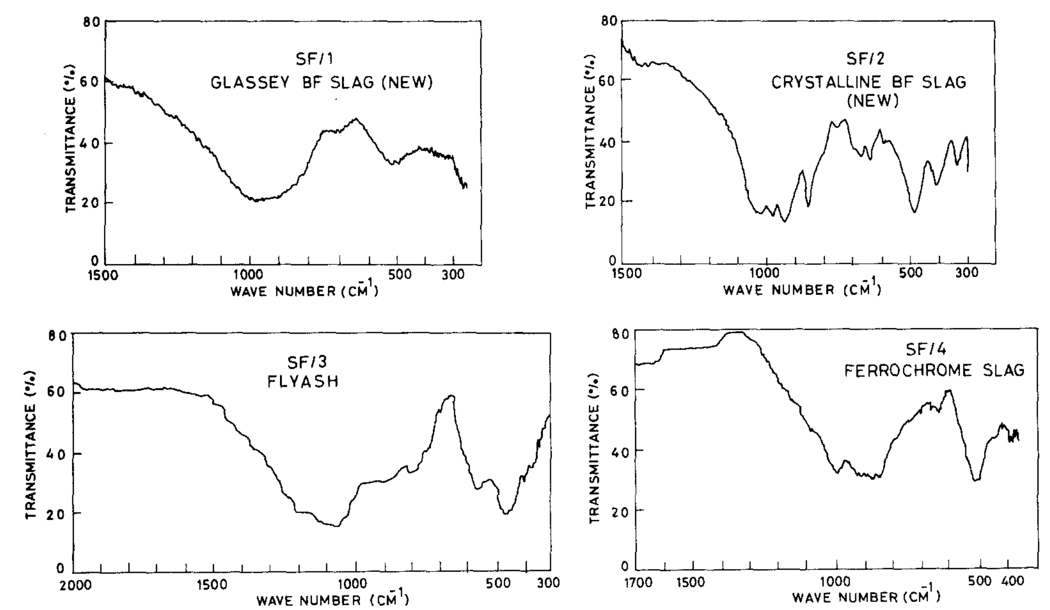


Figure 13 Spectra of slags and fly ash.

dicates the semi-crystalline nature of the material. The spectrum of the high alumina brick sample is poor. Several bands can, however, be located in its spectrum at 1150, 1100, 790, 730, 617, 555 and 460 cm^{-1}. The spectrum of the kyanite–sillimanite brick sample is very complex. The bands in the 1170 cm^{-1} region may be due to sillimanite [4]. Other regions of the spectrum are similar to kyanite. (Fig. 12)

3.9.1. Spectra of fly ash and slags

The spectrum of the fly ash sample is not well defined. The presence of bands in the region 800 to 600 cm^{-1} indicates quartz and the broad band in the 1100 cm^{-1} region can arise from the presence of sillimanite and mullite. The spectrum (SF/1, Fig. 13) of blast furnace slag indicates the amorphous nature of the material (broad bands) while the same slag crystallized in the laboratory shows the presence of melilite. The bands in the spectrum (SF/2, Fig. 13) closely resemble those of melilite [5]. The spectrum of the ferrochrome slag sample (SF/4, Fig. 13) shows the presence of β-Ca_2SiO_4 [6].

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