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FT-IR Spectroscopy Investigation of Soils From Yelagiri Hills, Tamil Nadu, India

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Abstract : FT-IR spectroscopy is a powerful tool for assessing the mineralogical composition of the soils. In the present study an attempt has been made to investigate soils of Yelagiri Hills, Tamilnadu India by Fourier transform infrared (FT-IR) spectroscopy. Qualitative analyses were carried out to determine the major and minor constituent minerals present in the samples from the band position or location of the peaks. From the prominent IR absorption peaks, the minerals identified with the available literature are quartz, microcline, orthoclase, kaolinite, montmorillonite, illite, and organic carbon. XRD confirms the presence of these minerals in soils. The interpretation of results is made from the characteristics of IR absorption bands. The results show that the FT-IR technique is a potential tool for the characterization of soil minerals.

Key words : Soil samples, FT-IR spectroscopy, Minerals.

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1. Introduction

Soil is a natural body consisting of layers (soil horizons) that are primarily composed of minerals mixed with at least some organic matter, which differ from their parent materials in their texture, structure, consistency, color, chemical, biological and other characteristics. It is the unconsolidated or loose covering of fine rock particles that covers the surface of the earth [1].Soils are heterogeneous, both laterally and vertically, and efficient land-resource assessment and soil management (such as "precision farming" concept) require accurate representation of this variability The principal constituents of most of the soils are quartz, feldspar, carbonates and clay minerals. Standard laboratory techniques for soil analysis are time-consuming and are not suitable for practical applications. Spectroscopy, both in the near infrared (NIR) and mid-infrared (MIR) ranges, is a promising technology for soil analysis [2-4].

Infrared techniques are most commonly developed for qualitative studies in mineral analysis. One of the most important and value added applications of the infrared spectroscopic study is the identification of the minerals in the soil samples. The Fourier Transform Infrared (FT-IR) absorption spectra of soils contain more information about mineralogy [6]. It is used by mineralogists and sedimentary petrologists in the aspect of mineralogical application. FT-IR techniques are used to distinguish the different types of clay minerals and to derive information concerning their structure, composition and structural changes upon chemical modification The present study was carried out to analyze the mineral composition of soil samples at various sites of Yelagiri Hills,Tamilnadu using FT-IR and XRD spectral analysis.

2. Materials and Methods

2.1. Sample Collection and Preparation

In the present study, soil samples were collected from four different locations of Yelagiri Hills,Tamilnadu, India using standard procedures [5]. The samples were collected at 50cm depth from the surface level. The samples were labelled as YS1, YS2, YS3, YS4.YS6,YS7, YS8,YS9,YS10,YS11 and YS12 The location maps are shown in Figure 1. These samples were dried at room temperature in open air for two days and stored in black polythene bags. The soil samples are ground well into a fine powder by using an agate mortar. The soil samples were well powdered and then oven dried at 60^0 C for 2 h to remove the moisture content and allowed to pass through sieves. This was done to maintain the grain size uniformity. The fine samples were used for mineral analysis.

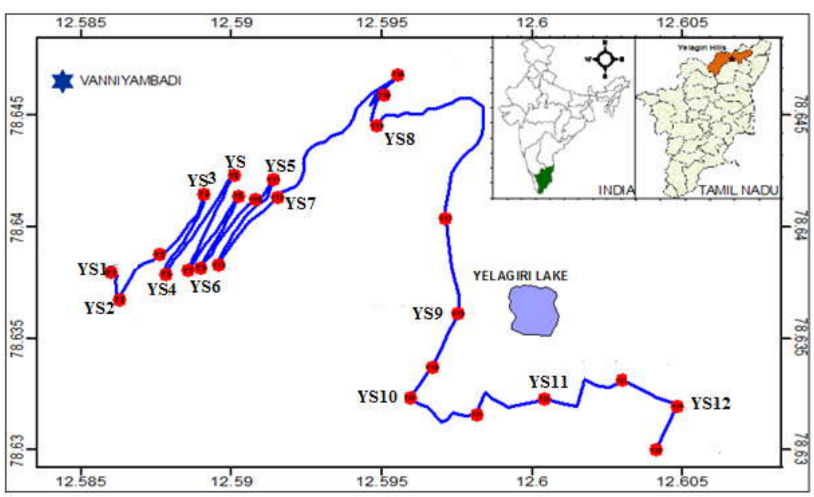

Figure 1 Location map of Yelagiri Hills, Tamilnadu

2.2. FT-IR Spectroscopy

The major and minor minerals are qualitatively determined by using FT-IR technique. The infrared spectra of the samples are recorded using KBr pellet technique in the region 4000–400cm^{-1}. The sample for irradiation is prepared by mixing the powdered sample with spectral grade KBr in the ratio of 1:20, KBr pellets having 13 mm diameter and 1 mm thickness are prepared under vacuum condition by applying a pressure of 10 torr on the stainless steel dies. The Perkin Elmer FT-IR spectrometer available in the Department of Chemistry, Muthurangam Government Arts College, Vellore; Tamilnadu, India is made use of in the present work for recording the FT-IR spectra of the samples at room temperature. A typical FT-IR spectrum as shown in Figure 2.

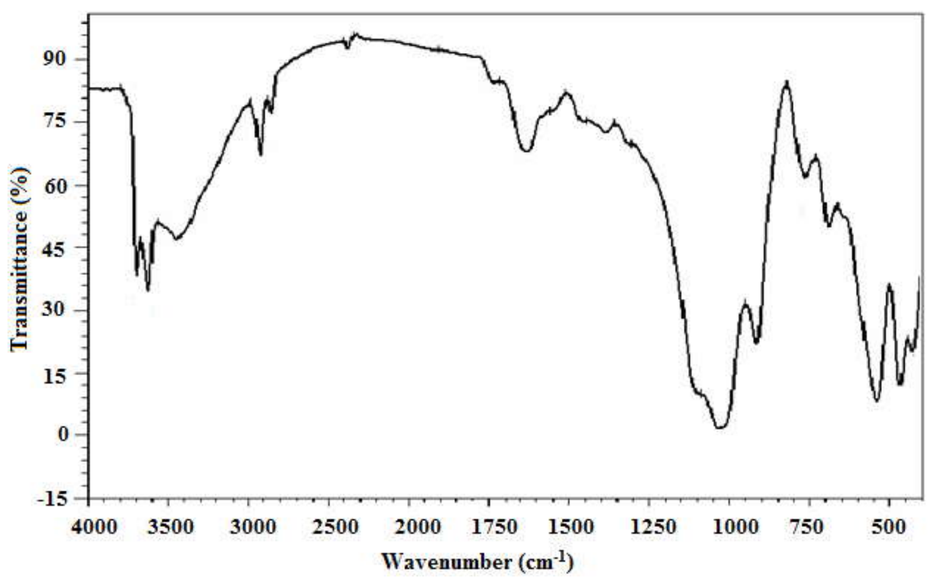

Figure 2. The typical FT-IR spectrum of soils of Yelagiri Hills,Tamilnadu.

2.3. X-ray Diffraction Technique

XRD is used to determine the mineralogical composition of the raw material components both qualitative and quantitative. The occurrences of minerals in soils were identified by comparing‘d’ values (Selected Powder Diffraction Data for Minerals 1974; Powder Diffraction File Search Manual Minerals 1974). No quantitative estimation phases in these adsorbents have been made but their characterization of XRD patterns indicates the presence of quartz, microcline, orthoclase, kaolinite, montmorillonite and illite, A typical XRD diffractrogram is shown in Figure 3.

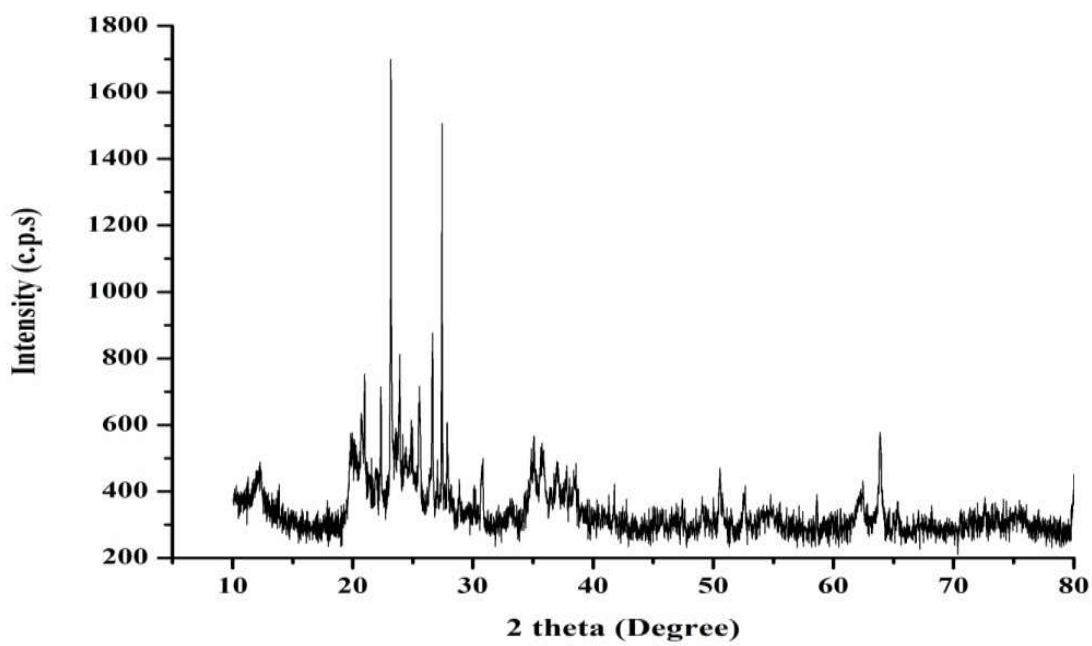

Figure 3. The typical XRD spectrum of soils of Yelagiri Hills,Tamilnadu.

3. Results and Discussions

The observed wave number unit (cm^{-1}) from all spectra are given in Table-1 along with their corresponding minerals and tentative assignments. By comparing the observed frequencies with the available literature, the minerals identified are quartz, microcline, orthoclase, kaolinite, montmorillonite, illite, and organic carbon [4-8].

Sample Locations												Tentative assignments	Minerals
YS1	YS2	YS3	YS4	YS5	YS6	YS7	YS8	YS9	YS 10	YS11	YS 12		
426	428	430	430	-	430	428	426	-	430	430	428	Si-O of Microcline	Microcline Feldspar
465	469	-	-	465	465	469	-	-	-	465	465	Si-O-Si bending	Orthoclase Feldspar
538	-	540	535	-		540	-	535	-	-	540	Si-O asymmetrical bending vibration	Orthoclase Feldspar
695	695	-	695	-	695	-	695	-	695	695	695	Si-O stretching	Quartz
-	775	775	775	775	775	775	775	775	775	775	775	Si-O stretching	Quartz
1090	-	-	-	1090	-	1095	-	1095	-	-	1095	Si-O stretching	Quartz
915	916	915	-	916	916	916	916	-	915	916	916	Al-O–H stretching	Illite
1035	1035	-	1030	1035	1030	1035	1035	1030	1030	1030	1035	Si-O stretching (Clay mineral)	Kaolinite
1635	1635	1635	1635	-	-	-	1635	1630	-	1635	1635	H-O-H stretching	Illite
-	1730	1730	-	-	-	1730	-		1730	-	1730	C=O band	Organic carbon
2855	2853	2855	2855	2856	2856	2856	2856	2856	2856	2856	2856	C-H stretching vibrations	Organic carbon
2925	-	-	2924	2924	2924	2924	2924	2926	2925	2926	2926	C-H stretching vibrations	Organic carbon
3440	-	-	3445	3445	-	-	3445	-	3445	-	3445	H-O-H stretching of water molecules	Montmorillonite
3620	3624	3622	-	-	-	3622	3624	-	-	3622	3625	O-H stretchg of inner hydroxyl group	Kaolinite
3690	-	-	3694	3694	3690	-	3694	3692	3692	3692	-	In Plane degeneratd vibration of the water molecule	Kaolinite

Table-1.The FT-IR spectral data of soils of mineral and their corresponding tentative assignment at various locations of Yelagiri Hills,Tamilnadu

3.1. FT-IR Spectroscopic Analysis

The FT-IR spectra indicate quartz and kaolinite as the major constituents and other minerals as the minor constituents. The mineralwise discussion is as follows.

3.2. Quartz

Quartz, one of the non-clay minerals, is common and invariably present in all the samples. It is the second most abundant mineral after feldspar, in the earth's crust. It is made up of a continuous framework of SiO_4 silicon–oxygen tetrahedra, with each oxygen being shared between two tetrahedra, giving an overall formula SiO_2. There are many different varieties of quartz, several of which are semi-precious gemstones. Throughout the world, varieties of quartz have been used in the making of jewellery and hard stone carvings.

The characteristic peaks of quartz are reported by several workers using FT-IR spectroscopic techniques [7-14]. IR observed frequencies at 695-700 cm^{-1}, 775-780cm^{-1} and 1090-1095 cm^{-1} shown in Table-1 suggest the presence of quartz. The strong absorption band observed at 695 cm^{-1} belongs to Si–O symmetrical bending vibration of quartz and the other one at 775cm^{-1} belongs to Si–O symmetrical stretching vibrations.

The peak appearing at 695 cm^{-1} is most useful to determine nature of the mineral with regard to the structural stability. Many workers have calculated the crystallinity index of quartz using the symmetrical bending vibration of Si-O group obtained at 695 cm^{-1}. The 695 cm^{-1} is present in the spectra of the sample indicate quartz mineral are well in crystalline form.

3.3. Feldspar Minerals

Feldspar is a blanket term for a very large group of minerals which are extremely abundant on Earth. Around 60% of the Earth's crust is made up of feldspar; the feldspars are a group of minerals that have similar characteristics due to a similar structure. The general formula, for the common feldspars, is XAl (1-2) Si (3-2) O_8. The X in the formula can be sodium, Na and/or potassium, K and/or calcium, Ca. The distinguishing feature of minerals in the feldspar group is that they are comprised of silicates of aluminium blended with other metals like potassium, calcium, sodium, and sometimes barium. The composition of an individual piece of feldspar determines its chemical properties and what colour it will be, but it shares similarities with other feldspars, like crystalline structure

From Table-1, IR observed frequencies at 425-430 cm^{-1}, 465-470 cm^{-1} 535-540cm^{-1} and indicates the presence of feldspars in the all the samples [5-8]. The peaks at 465-470cm^{-1} and

535-540cm^{-1} belong to Si-O-Si bending and Si-O asymmetrical bending vibration and it indicates the presence of orthoclase in all the samples [11]. The peak observed at 420-425 cm^{-1} is ofmicrocline.

3.4. Clay Minerals

Clay minerals are hydrous aluminium phyllosilicates, sometimes with variable amounts of iron, magnesium, alkali metals, alkaline earths, and other cations. Clays have structures similar to the micas and therefore form flat hexagonal sheets. Clay minerals are common weathering products (including weathering of feldspar) and low temperature hydrothermal alteration products. Clay minerals are very common in fine grained sedimentary rocks such as shale, mudstone, and siltstone and in fine grained metamorphic slate and phyllite. Clay minerals include Kaolin group which includes the minerals kaolinite, dickite, halloysite, and nacrite (polymorphs of $Al_2Si_2O_5(OH)_4$) and Smectite group which includes dioctahedral smectites such as montmorillonite and nontronite and trioctahedral smectites for example saponite. The clay minerals (kaolinite and montmorillonite) are present variably in the samples under investigations as is evidenced from the Table-1. Kaolinite is the major constituent of clays which gives sharp absorption bands in the 3700–3600 cm^{1} region.

Strong bands between 3690-3695cm^{-1} indicate the possibility of the hydroxyl linkage. However, absorption band 3620-3625cm^{-1} in the spectrum of samples suggests the possibility of water of hydration in the adsorbent. The observed frequencies 3690 cm^{1}, 3620 cm^{-1} and 1030 cm^{-1} are attributed to kaolinite. The broad absorption band observed at 1030 cm^{1} belongs to Si–O stretching of kaolinite (clay mineral) [12-14].

The observed strong absorption frequencies in the range of 3440-3445cm^{-1} in the spectrum of clay suggests the possibility of H-O-H stretching of water molecules. Peaks appearing at

3440- 3445cm^{-1} in the samples show the presence of montomorillinte [12-14]. Illite and kaolinite are the main clay minerals which are more common in soils and in natural aerosols. The observed strong absorption frequency at 1635 cm^{-1} in the spectrum of samples suggests the possibility of water of hydration in the adsorbent. The frequencies observed at 1635 and 915cm^{-1} indicate the possibility of the presence of illite [14-15]. The band at study 915cm^{-1} is due to Al-O–H stretching vibration.

3.5. Organic Carbon

From the spectra of all the samples, a very weak to weak absorption bands present at 2920-2925 and 2850-2855 cm^{-1} may suggest the presence of organic carbon [15-16]. These bands are due to C-H absorption contaminants present in the samples. Another peak 1730cm^{-1} is for YS2 and YS3 shows the presence of organic carbon .This band belongs to carbon and oxygen double bonded linkage (C=O) .

4. X-ray Diffraction Analysis

Qualitative mineralogy of the soil samples was determined with the standard interpretation procedures of XRD. Quartz, albite, orthoclase, microcline, calcite, illite and kaolinite, were identified from the peaks in diffractrogram. Major minerals in the samples are quartz and feldspars. The FT-IR findings are confirmed by XRD analysis and it reveals that these techniques are used for mineral analysis.

5. Conclusion

The FT-IR analyses of soil samples collected from different locations of Yelagiri Hills, Tamilnadu indicate the presence of quartz, microcline, orthoclase, kaoillinte, montomorillinte, illite and organic carbon. Among the different minerals quartz, feldspar and kaolinite are present invariably in all soils. Hence, they are considered to be main or major constituent of the soil and feldspar is present in different compositions. This is also confirmed by XRD-technique. Hence both FT-IR and XRD method are promising tools for mineral analysis in soil samples.

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