Mineral Characterization and Crystalline Nature of Quartz in Ponnaiyar River Sediments, Tamilnadu, India

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Abstract: Mineral characterization of sediment samples collected from Ponnaiyar River at various sites is carried out using Fourier Transform Infrared (FTIR) spectroscopic technique. The obtained result from this study shows the presence of quartz, feldspar in different structure, kaolinite as major minerals. The other minerals such as calcite, gibbsite, montmorillonite, smectite, organic carbon and polygorskite are as minor minerals. The relative distribution of major minerals such as quartz, feldspar (orthoclase and microcline) and kaolinite are determined by calculating extinction co-efficient. The crystalline nature of quartz in various sites is studied by calculating crystallinity index. The obtained results from both calculations are presented and discussed.

Key words: FTIR · Minerals · River sediments · Extinction co-efficient · Crystallinity index

INTRODUCTION

The Fourier Transform Infrared (FTIR) absorption spectra of sediments contain more information about mineralogy [1ss]. It is used by mineralogists and sedimentary petrologists in the aspect of mineralogical application. Sediments are detrital products of rocks and bear the mineralogical properties of the original rock formation. The principal constituents of most of the sediments are quartz, feldspar, carbonates and clay minerals. Of these, quartz is overwhelmingly the most abundant. Feldspar, though more abundant in parent igneous rock, is of intermediate durability and so runs second place to quartz in sediments. The others, though more durable than feldspar, are simply for less abundant in source materials [2]. The mineralogical properties of sediments, reflects the geological history of transport and sorting process. Moreover, the scientific studies of the identification of minerals in sediments lead to useful information about possible origin of minerals. So the characterization of minerals in sediments plays a vital role in research. The Infrared spectra of river sediments from Cauvery and Vellar have been characterized by

Hence, the main scope of this study is to identify and characterize the various minerals present in river sediments by FTIR technique. Also to study, the crystalline nature of quartz present in the sediments.

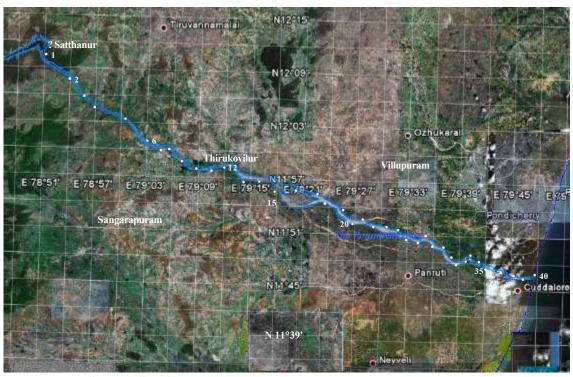
Ramasamy *et al.* [1, 3].

MATERIALS AND METHODS

Study Area: In the present investigation, sediment samples were collected from various sites of the Ponnaiyar river (Fig. 1). It is originated on the hills of Nandidrug in Kolar districts of Karnataka state and flows south and then east for 400Km through Karnataka and Tamilnadu and terminated at Cuddalore, Tamilnadu in Bay of Bengal. It is entered in Tamilnadu at Dharmapuri district. It covers four districts (Dharmapuri, Thiruvannamalai, Villupuram and Cuddalore) in Tamilnadu. A dam is constructed on this river at Satthanur, Chengam taluk, Thiruvannamalai district. Capacity of this dam nearly 4600 M CFT. The sediments of this river are excavated only for building constructions.

Sample Collection and Preparation: The present study area (Ponnaiyar river) covers a total length of 200 Km, from which 40 locations were selected. Each location is separated by a distance of 4-5 Km approximately. All sediment samples were collected at 0-10 cm depth during the summer season (April-May 2008). Each sample has a weight of 3-4 kg approximately. The collected samples were dried at room temperature in open air for two days and stored in black polythene bags.

Wet grinding was carried out by placing 30 to 50mg of the sample in an agate mortar along with 20 to 25 drops of ethanol. The ground samples were dried in a hot air oven at 110°C to remove the moisture content and sieved



•-represents successive sampling sites

Fig. 1: Location of Ponnaiyar river with their experimental sites in Tamilnadu

to various grain sizes such as 74, 53 and 44im. Using the KBr pellet technique, each grain sized sample was mixed with KBr at various ratios viz., 1:10, 1:20, 1:30, 1:40 and 1:50. The mixture was then pressed into a transparent disc in an evacuable dye at sufficiently high pressure. The samples in the ratio 1:30 was taken for further analysis, since it gives rise to maximum transmittance and observable peaks [1]. Using the Perkin Elmer RX1 FTIR spectrometer, the infrared spectra for all sediment samples were recorded in the region 4000-400 cm⁻¹. The resolution of the instruments is 0.001cm⁻¹ and the accuracy is 4 cm⁻¹.

RESULTS AND DISCUSSION

The infrared spectra of all sediment samples collected from various sites of Ponnaiyar river are recorded and their frequencies (cm⁻¹) obtained from these spectra are tabulated with corresponding minerals in Table 1. Comparing these observed frequencies with those available literatures [1, 3-5], the minerals such as quartz, microcline feldspar, orthoclase feldspar, kaolinite, calcite, gibbsite, montmorillonite, smectite, organic carbon and polygorskite are identified.

Among these minerals, quartz is invariably present in all samples. It is one of the non clay mineral. The presence of quartz in the samples can be explained by Si-O asymmetrical bending vibrations around 464 cm⁻¹, Si-O symmetrical bending vibrations around 694 cm⁻¹, Si-O symmetrical stretching vibrations at around 778 and 796 cm⁻¹, while the 1082 and 1162 cm⁻¹ absorption region arises from Si-O asymmetrical stretching vibrations due to low Al for Si substitution. The observation of peaks near 514-520 cm⁻¹ also indicates that presence of Quartz. With the view of Keller and Pickett [6], the observed absorption peaks at 1615-1620 cm⁻¹ in some sites indicate the presence of quartz in river sediments are weathered from metamorphic origin. These assignments are in good agreement with the observation on the quartz mineral obtained by Ramasamy et al. [1, 3, 5]. The characteristic feature of quartz is a doublet centered at or around 796 and 778 cm⁻¹. Usually, the intensities of the above doublet are not comparable.

Feldspar is also frequent constituents in sediments. This group of minerals are of several types such as orthoclase, microcline, sanidine (K-feldspar), albite (Na-feldspar) and anorthite (Ca-feldspar). Though three feldspars (orthoclase, microcline and sanidine) are having

Table 1: The observed absorption wave numbers and corresponding minerals from FTIR spectra

S. No.	Mineral Name	Site number	Observed Wave numbers (cm ⁻¹)
1	Quartz	S ₁ -S ₄₀	460-464
		S_1-S_{40}	514-520
		S_1-S_{40}	693-694
		S_1 - S_{40}	777-778
		S_1 - S_{40}	794-796
		S_1 - S_{40}	1080-1084
		S_1 - S_{40}	1162-1164
		S_6, S_9, S_{13} - $S_{19}, S_{22}, S_{31}, S_{35}$ - S_{37}	1615-1620
2	Microcline Feldspar	$S_1 - S_{40}$	583-587
3	Orthoclase Feldspar	S_1 - S_{40}	647-650
		$S_1, S_3, S_{15}, S_{21}, S_{23}, S_{29}$	532-537
4	Kaolinite	S_1 - S_{40}	1015-1019
		S_1, S_3, S_{10}, S_{15}	1030-1037
		$S_6, S_{10}, S_{15} - S_{19}, S_{24}, S_{32}, S_{35} - S_{36}$	3618-3622
		$S_{6},S_{9},S_{13}\text{-}S_{19},S_{22},S_{31},S_{35}\text{-}S_{37}\\ S_{1}\text{-}S_{40}\\ S_{1}\text{-}S_{40}\\ S_{1},S_{3},S_{15},S_{21},S_{23},S_{29}\\ S_{1}\text{-}S_{40}\\ S_{1},S_{3},S_{10},S_{15}\\ S_{6},S_{10},S_{15}\text{-}S_{19},S_{24},S_{32},S_{35}\text{-}S_{36}\\ S_{1},S_{2},S_{23},S_{33},S_{29},S_{34}\\ S_{1}\text{-}S_{40}\\ S_{2},S_{3},S_{4},S_{33},S_{36}\\ S_{36}$	3690-3691
5	Gibbsite	S_1 - S_{40}	662-670
6	Calcite	S ₂ , S ₃ , S ₄ , S ₃₃ , S ₃₆	1420-1438
7	Montmorillonite	S_{36}	878
8	Polygorskite	$S_1, S_7, S_{21}, S_{33}, S_{29}, S_{36}$	3611-3615
9	Organic Carbon	S_1 - S_{40}	2923-2929
		S_1 - S_{40}	2852-2865
10	Smectite	S_{27}	523

the same chemical formula (KAlSi $_3$ O $_8$) but they have different structures (orthoclase-monocline, microcline-triclinic and sanidine-tetrahedral). The peak corresponding the range 583-587 cm $^{-1}$ is due to the O-Si-(Al)-O bending vibration for microcline and in the range 647-650 and 532-537cm $^{-1}$ is due to the Al-O coordination vibrations indicates the presence of orthoclase feldspar [1].

Kaolinite is the clay mineral. The presence of absorption band at or around 3690, 3620, 1030 and 1015 cm⁻¹ indicate the presence of clay mineral constituents as kaolinite [1, 4]. The intensity of the bands varies from sample to sample which indicates its the quantity. According to Russell [4] and Ramasamy *et al.* [3], if four peaks are observed in the region 3697-3620 cm⁻¹, the minerals are said to be ordered state. However, in the present study only two peaks are observed at 3690 and 3620 cm⁻¹ in some sites. This suggests the minerals may be in disorder state.

Calcite is the most common carbonate mineral in sediments. From the existence of a peak in the range 1420-1438 cm⁻¹ it is easily recognized that the calcite is present in site no. S₂-S₄, S₃₃ and S₃₆. The existence of a peak near 665, 878, 523, 2925 and 2855 and 3612 cm⁻¹ respectively indicate that presence of gibbsite, montmorillonite, smectite, organic Carbon and polygorskite.

Extinction Co-efficient of Quartz, Feldspar (Orthoclase and Microcline) and Kaolinite: The relative distribution of major minerals can be quantified by calculating the extinction co-efficient. With reference to the number of peaks and intensity, the minerals such as quartz, feldspar (orthoclase and microcline) and kaolinite are consider as major or main minerals. The other minerals are accessory. Therefore in the present study, the author is interested to study the relative distribution of quartz, feldspar (orthoclase and microcline) and kaolinite in Ponnaiyar river sediments. The characteristic peaks of quartz, orthoclase feldspar, microcline feldspar and kaolinite at around 778,647,585 and 1015 cm⁻¹ respectively are taken for calculation using the formula [7].

K = DA/M

Where K is the extinction coefficient, D is the optical density, A is the area of the pellet and M is the mass of the pellet. From the calculated values (Fig. 2), maximum extinction co-efficient values for quartz, microcline feldspar, orthoclase feldspar and kaolinite are 275.75, 46.43, 27.36 and 5.16 in the site no. S₂₅, S₁₈, S₂₅ and S₄₀ respectively. In the same way, minimum values are 35.68, 6.65, 3.38 and 1.10 in the site no. S₃₆, S₂₈, S₂ and S₁ respectively. With the maximum and minimum limits of the above said minerals, the other sites may be arranged for

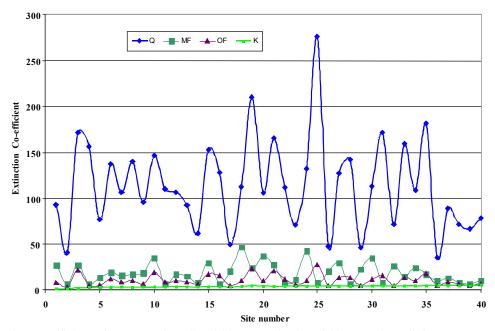


Fig. 2: Extinction co-efficient of Quartz, Microcline feldspar, Orthoclase feldspar and Kaolinite

the containment of the same mineral quantitatively in an order. In overall view, the amount of kaolinite is very much lesser than quartz and lesser than orthoclase and microcline feldspar.

Crystallinity Index of Quartz: Crystallinity can be defined as fraction of crystalline materials in a mixture of crystalline and non-crystalline materials. The crystallinity index is inversely proportional to crystallinity. Since quartz is the major mineral present in the sediment samples, the crystallinity index of quartz has been calculated. The crystallinity of quartz will give a clear indication on the crystalline forms of other minerals because quartz is the mineral, which crystallizes last. Hence, it is useful to find out the crystallinity of quartz rather than the other minerals.

The crystallinity index is calculated by taking the ratio of the intensity of absorption band at around 777 cm $^{-1}$ (I $_{777}$) to the band at around 695cm $^{-1}$ (I $_{695}$) using the tangent base line method [8]. When crystallinity index is minimum, the minerals are said to be in well crystallized state and if it is maximum, the minerals are considered to be in poorly crystallized state.

From the calculated crystallinity index (Table 2), it is found that the site S_2 , S_{14} , S_{17} , S_{36} and S_{38} - S_{40} are having the higher crystallinity index, which shows low degree of crystalline nature of quartz. Site number S_1 , S_5 - S_9 , S_{11} - S_{13} , S_{16} , S_{18} , S_{29} , S_{30} , S_{37} and S_{38} have intermediate structure of quartz. Site number S_3 , S_4 , S_{10} , S_{15} , S_{19} - S_{28} and

Table 2: The Crystallinity index of quartz in all sites

Site	Crystallinity	Site	Crystallinity
number	index	number	index
$\overline{S_1}$	0.7800	S_{21}	0.6444
S_2	0.9051	S_{22}	0.6759
S_3	0.6439	S_{23}	0.6225
S_4	0.6894	S_{24}	0.6541
S_5	0.7935	S_{25}	0.5045
S_6	0.7185	S_{26}	0.6340
S_7	0.7676	S_{27}	0.6623
S_8	0.7090	S_{28}	0.6857
S_9	0.7823	S_{29}	0.7516
S_{10}	0.6940	S_{30}	0.7639
S_{11}	0.7698	S_{31}	0.6439
S_{12}	0.7676	S_{32}	0.6507
S_{13}	0.7931	S_{33}	0.6742
S_{14}	0.8667	S_{34}	0.5676
S_{15}	0.6791	S_{35}	0.6378
S_{16}	0.7163	S ₃₆	0.8650
S_{17}	0.8896	S_{37}	0.7516
S_{18}	0.7483	S_{38}	0.8446
S ₁₉	0.5840	S_{39}	0.8533
S_{20}	0.6897	S_{40}	0.8345

 S_{31} - S_{35} have lower crystallinity index, which shows higher order crystalline nature. Especially, site number S_{19} , S_{25} and S_{34} have well ordered crystalline quartz because these sites have lower crystallinity index value.

CONCLUSION

The present study indicates that the presences of minerals such as quartz, feldspar (orthoclase and microcline) and kaolinite as major minerals. The others such as calcite, gibbsite, smectite, montmorillonite, polygorskite and organic carbons are considered as minor minerals. Among the different minerals, quartz, feldspar (orthoclase and microcline) and kaolinite is present in all samples. Hence, these minerals are considered to be main or major constituents of the samples. The observed absorption peaks at 1615-1620 cm⁻¹ in some sites indicate the presence of quartz in river sediments are weathered from metamorphic origin. The calculated extinction coefficient values show that, the amount of quartz is greater than feldspar (orthoclase and microcline) and very much greater than kaolinite in all the sites. The observation of results from crystallinity index shows that the low degree of crystalline nature of quartz is observed at S_2 , S_{14} , S_{17} , S_{36} and S_{38} - S_{40} . Site number S_3 , S_4 , S_{10} , S_{15} , S_{19} - S_{28} and S_{31} -S₃₅ have higher order crystalline quartz. Among this, well ordered crystalline quartz is observed at S_{19} , S_{25} and S_{34}

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