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STRUCTURAL AND OPTICAL CHARACTERISTICS OF SODIUM NITRATE AND LITHIUM SULPHATE MONOHYDRATE WITH SODIUM NITRATE SINGLE CRYSTALS

*Anithalaksmi M¹, Robert R*², Jayanthi G³*

^{1&3}Department of Physics, Adhiyaman Arts and Science College for Women,

Uthangarai, Krishnagiri – 635 207

²Department of Physics, Government Arts College for Men, Krishnagiri – 635 001

*E-mail: roberthosur@yahoo.co.in, Tel: 9443982828

ABSTRACT

The sodium nitrate and Lithium Sulphate Monohydrate Sodium Nitrate single crystals were grown by slow evaporation technique at room temperature. The grown crystals were subjected to powder X-ray diffraction and that confirms quality of these two crystals. The Fourier Transform Infrared Spectroscopy ensures the functional group of the grown sample, the optical transparency was judged based on the UV-Visible spectral analysis and cut-off wavelength of the crystal were calculated from the UV- Visible transmission spectra.

Keywords: Powder X-ray diffraction, FTIR, optical transparency, UV-Visible Spectroscopy.

1. INTRODUCTION:

Crystal growth is one of the most important fields of material science, which involves controlled phase transformation. Fundamental experimental aspects of crystal growth were derived from early crystallization in the Eighteenth and Nineteenth century. The phenomena of under cooling super saturation and the heat of crystallization were recognized in the Eighteenth century. Theoretical understanding started with the development of nucleation and crystal growth theories[1]. The critical one to achieve higher quality crystal and

the role of transport phenomena was a unique feature of the twentieth century. In the past, there was a growing interest in crystal growth process, particularly in view of the increasing demand for materials for technological application. Therefore, researchers worldwide have always been in search of new materials through their single crystal growth. The methods of growing crystals are very wide and mainly dictated by the characteristics of the material and its size[2].

2. EXPERIMENTAL PROCEDURE:

In this crystal growth process the sodium nitrate grown by slow evaporation method. Being by making a saturate solution of sodium nitrate. 0.8499g of sodium nitrate is dissolved in 10 ml of water, The solution is stirred slowly until all the salt has been dissolved in the solvent. Stirring process was taken place for 3 hour. A crystal of lithium sulphate monohydrate and sodium nitrate were grown at room Temperature by the reaction between lithium sulphate monohydrate and sodium nitrate and dissolving 1 mol % of $\text{Li}_2\text{SO}_4 \cdot \text{H}_2\text{O}$ with 1mol % of NaNH_4 in distilled water. The solution was Continuously stirred well for 4 hours using a magnetic stirrer. and the solution is filtered by whatman filter paper[3-5]. The filtered solution was transferred into the two separate beaker and covered with perforated polythene sheet, so that the solution would evaporate slowly. The grown process was carried out in a room temperature.

The nucleation process of sodium nitrate being within 6 days and the seed of the grown crystal were observed. The sizes of the crystals are varied with the interaction of seed force of attraction, later of 3 weeks the crystal was harvested within the size of 7mm x 4mm x 1mm as shown in fig 1.a. The solution of lithium sulphate monohydrate and sodium nitrate was allowed to evaporated at room temperature, tiny seed were observed within 12 days and good quality crystals in the size of 10mm x 6mm x 2mm were grown in 3 weeks as shown in below fig 1.b.

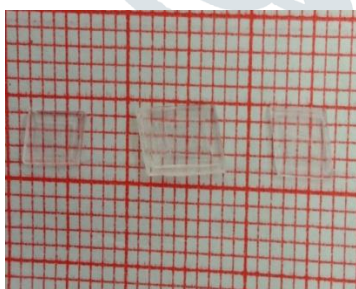


Fig 1.a

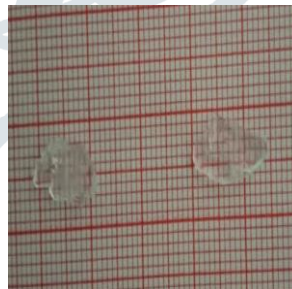


Fig 1.b

Fig.(1.a & 1.b) Structure of Sodium Nitrate and Lithium Sulphate Monohydrate Sodium Nitrate

3. RESULTS AND DISCUSSION:

3.1 Powder X-ray Diffraction Analysis:

The powder form of the grown crystals were subjected to powder X-ray diffraction analysis. The X-ray diffraction data were recorded using monochromatic CuK α -1 radiation of wavelength 1.54060(A) recorded between 2θ ranging from 0° to 100° as shown in fig 2.a. The diffraction pattern contains various reflections corresponding to various crystallographic planes in between the angles 10° to 80° . The narrow peak at hkl plane (104) in the XRD pattern show the good quality crystalline nature of the grown crystals. The data obtained is good agreement with standard JCPDS file (JCPDS 77-1900) of sodium nitrate single crystal. The reflection planes were indexed in accordance with the JCPDS file[6]. From powder X-ray diffraction analysis, it has been confirmed that the grown pure sodium nitrate crystal belongs to rhombohedral system. The narrow peak in the lithium sulphate monohydrate and sodium nitrate XRD pattern show the good quality crystalline nature of grown crystal. The mixing of these composition of lithium sulphate crystal increases the intensity of peaks comparing to pure lithium sulphate monohydrate crystal[7-9]. The doping has brought a change in the internal structure of crystal. From powder X-ray diffraction analysis it has been confirmed that grown lithium sulphate monohydrate with sodium nitrate crystal belongs to Orthorhombic system.

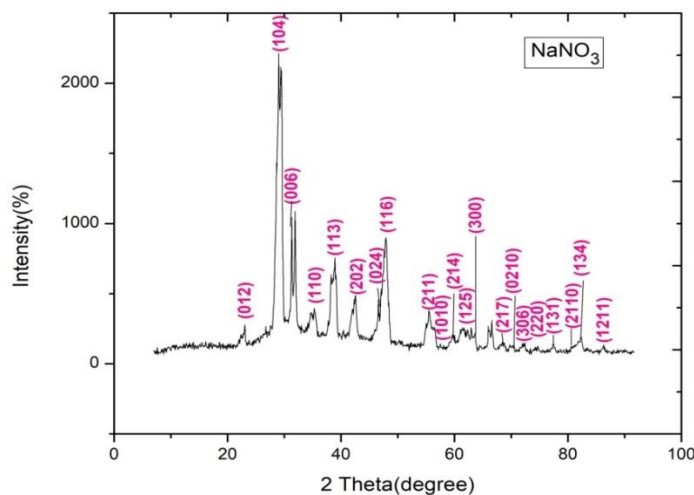


Fig 2.a Powder X-ray diffraction pattern of pure Sodium Nitrate single crystal.

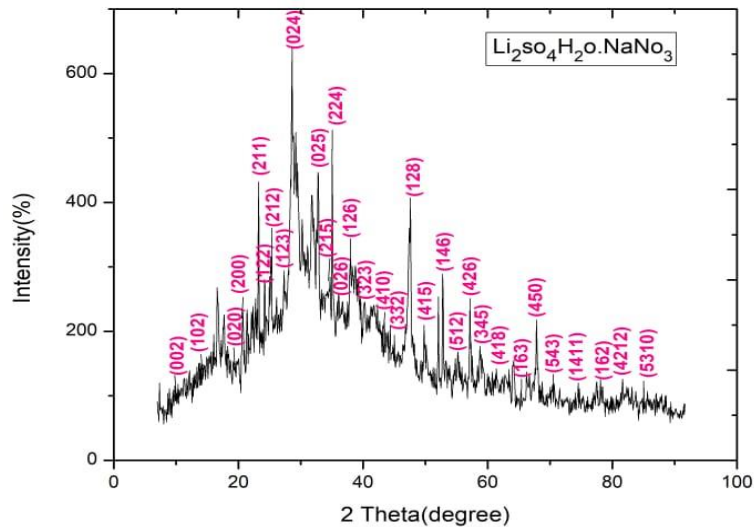


Fig 2.b. Powder X-ray diffraction pattern of Lithium Sulphate Monohydrate with Sodium Nitrate.

3.2. Fourier Transform Infrared (FTIR) Analysis:

Fourier Transform Infrared spectral analysis is one of the most prominent and broadly used spectroscopic methods for analyzing the structure of unknown compounds quantitatively. It is useful to find out the functional groups presents in the internal structure of the molecules and the nature chemical bonds of a compound[10-12]. The Fourier Transform Infrared spectra of pure sodium nitrate crystal and lithium sulphate monohydrate and sodium nitrate crystal were recorded in the range of 400–4000 cm^{-1} , were shown in fig 3.a and 3.b respectively. For pure sodium nitrate single crystal the band at 2828 cm^{-1} assigned to stretching vibration of O-H group[12-15]. The bending vibration mode of O-H group is identified at 2426 cm^{-1} . The stretching vibration mode of S-O group found at 818 cm^{-1} . Numerous aspects such as stretching, contraction of bonds in the interaction of stretching modes might be involved in the compression of the peak areas of the composites.

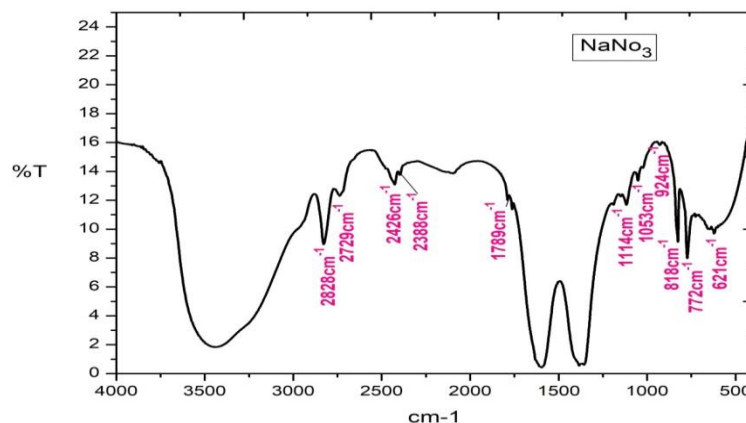


Fig 3.a. FTIR Spectrum of Sodium Nitrate.

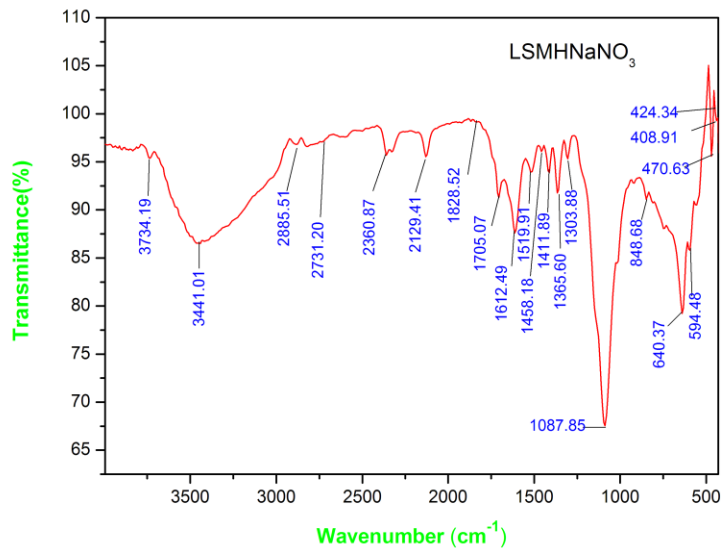


Fig 3.b. FTIR Spectrum of Lithium Sulphate Monohydrate with Sodium Nitrate.

3.3.UV – Visible Spectral Analysis:

The UV – Visible transmission spectra of pure sodium nitrate and lithium sulphate monohydrate with sodium nitrate and crystal were recorded by using systronics double beam spectrophotometer -2201 in the wavelength range 200 – 800nm[16]. The spectra were shown in fig 4.a. and 4.b respectively. From the UV – Visible transmission spectrum of sodium nitrate, the transmittance is more than 90% in the entire visible region and the cut-off wavelength lies near 260nm. The band gap value of sodium nitrate crystal was found out using the relation $[E=hc/\lambda]$ and is found to be $E_g = 4.76$ eV. The cut-off wavelength of lithium sulphate monohydrate with sodium nitrate were lies near 279 nm. The band gap value of this crystal was found to be $E_g=4.44$ eV.

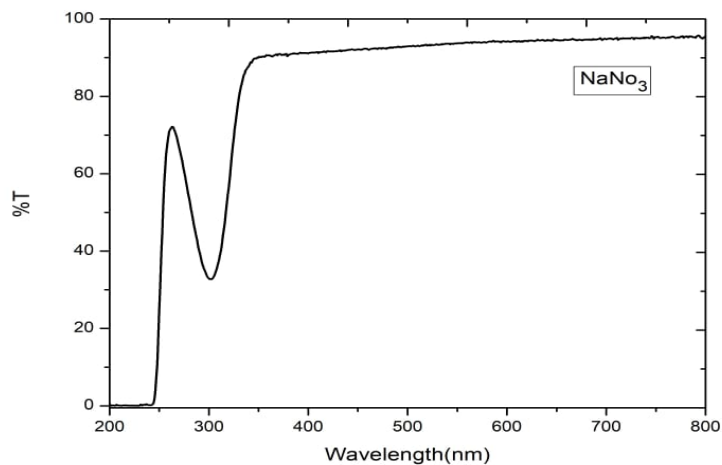


Fig 4.a UV – Visible transmission Spectrum of Sodium Nitrate.

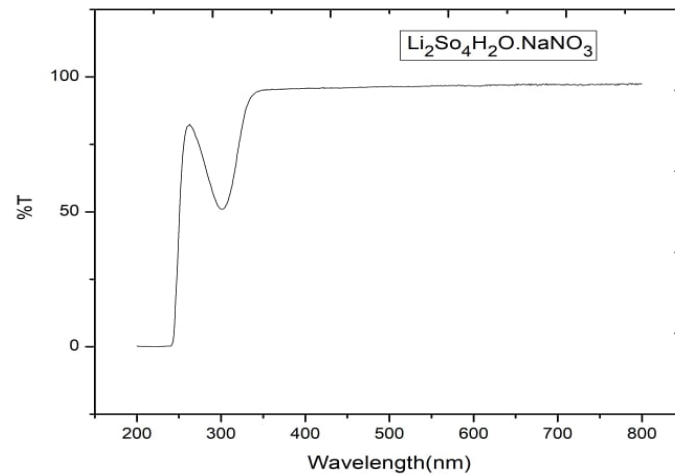


Fig 4.b UV – Visible transmission Spectrum of Lithium Sulphate Monohydrate with Sodium Nitrate.

4. CONCLUSION:

The single crystal of pure Sodium Nitrate and Lithium Sulphate Monohydrate with Sodium Nitrate were grown by slow evaporation method. The powder X-ray diffraction analysis revealed that the sodium nitrate crystal belongs to rhombohedral system and lithium sulphate monohydrate with sodium nitrate crystal belongs to orthorhombic system. The vibrational modes of functional groups were identified using FTIR spectroscopic technique. From the UV-Visible spectrum of both sodium nitrate and lithium sulphate monohydrate with sodium nitrate had the energy band gaps 4.76eV and 4.44eV respectively. Hence these crystals may be useful to make optoelectronic devices.

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