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Growth and Characterization of Sodium Sulphate Doped L-Alanine Crystal

M. Abila Jeba Queen[1], K.C.Bright[2], S. Mary Delphine[1]

[1] Research Department of Physics, Holy Cross College (Autonomous), Nagercoil-629004, Tamil Nadu, India.
(Affiliated to Manonmaniam Sundaranar University, Abishekapatti, Tirunelveli-627012, Tamil Nadu, India)
[2] Department of Physics, St. John's College, Anchal-691306, Kerala, India.

ABSTRACT

Sodium sulphate doped L-Alanine single crystals were grown from aqueous solution by slow evaporation technique. The grown crystals were subjected to powder X-ray diffraction analysis, to confirm the crystalline nature of the crystal. The lattice parameters were found out using single crystal X-ray diffraction. To identify the functional groups Fourier transform infrared analysis was taken.

Keywords: L-Alanine, Sodium sulphate, Powder X-ray diffraction, FTIR.

1. Introduction

In photonics pertaining process nonlinear optical materials plays an important role. The major applications are information processing, optical data storage, telecommunication sensor protector etc. In many cases organic compounds exhibit large response. It offers the flexibility of molecular design and the promise of virtually an ultimate number of crystalline structures. In this emerging context organic non linear materials have been recognized as a forefront candidate for fundamental and applied investigations including the joint effort of chemists, material scientists and optical engineers [1-5]. Amino acid crystals have good NLO applications including proton donating and proton accepting group. In this work we report the growth of sodium sulphate doped L-Alanine single crystal. The grown crystals were characterized by PXRD, Single Crystal XRD and FTIR studies.

2. Experimental Procedures

Crystals of sodium sulphate doped L-Alanine were grown by slow evaporation method. The solution was prepared by dissolving L-Alanine and sodium sulphate in the mole percentage ratio 1 : 0.1. Since the mixture is readily soluble in water, deionised water is used as the solvent. Nucleation occurred after 7days. Good quality crystals are harvested after 20 days. The photograph of the grown crystal is shown below.

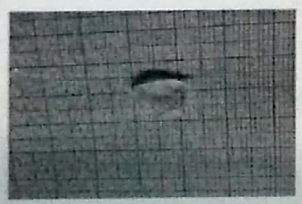

Figure:1. Photography of grown Sodium sulphate doped L-Alanine crystal

3. Result and Discussion

The grown crystal was characterized by powder X-ray diffraction studies to confirm the crystalline nature. Single crystal X-ray diffraction studies were carried out to find the crystal structure and Fourier transform infrared spectroscopy is effectively used to identify the functional groups.

3.1. X-Ray Powder Diffraction Analysis

The crystalline nature of sodium sulphate doped L-alanine single crystal was studied by powder X-ray diffraction method. Powder XRD patterns of the grown crystals were recorded using the X-ray diffractometer PAN Analytical XPERT-PRO. The intensity of the diffracted beam against 2θ is recorded in the range 10-80^0 with Cuk$_\alpha$ radiation (λ=1.54056Å). Using the observed 2θ (Bragg angle) and d spacing all the reflections of the powder XRD pattern for L-Alanine sodium sulphate crystal has been indexed using the "INDEXING" software packages. The indexed X-ray powder diffraction patterns of the grown crystal are show in figure 2. The sharp peaks confirmed the crystalline nature and purity of the crystal.

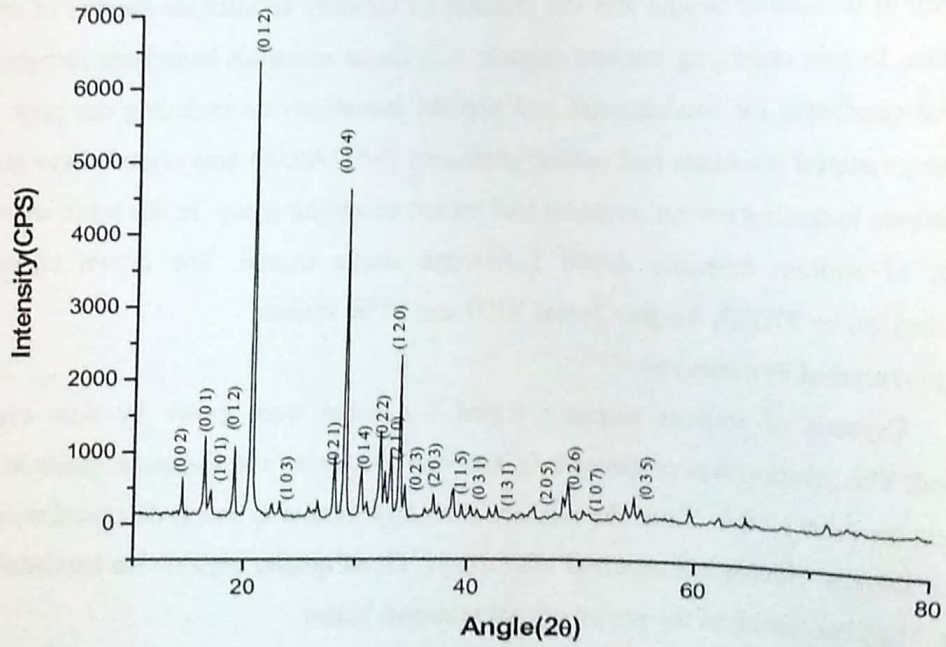

Figure:2. XRD pattern of Sodium sulphate doped L-Alanine crystal

3.2. Single Crystal X-Ray Diffraction

Single crystal X-ray diffraction studies of sodium sulphate doped L-Alanine crystal was carried out using Bruker Kappa Apex II diffractometer. From the data, it was found that the crystal belongs to orthorhombic system with a = 5.808Å, b = 6.049 Å, c = 12.38Å , $\alpha = \beta = \gamma = 90^0$ and volume 435Å^3. When sodium sulphate has doped with L-Alanine a small variation in the lattice parameter values were obtained.

3.3.FTIR Analysis

Fourier transform infrared (FTIR) spectra were recorded in the frequency range 400-4000 cm^{-1} using the Perkin Elmer Spectrometer. The Fourier infrared spectrometer is effectively used to identify the functional groups present in the sample. The FTIR spectra of sodium sulphate doped L-Alanine crystal was shown in figure 3.

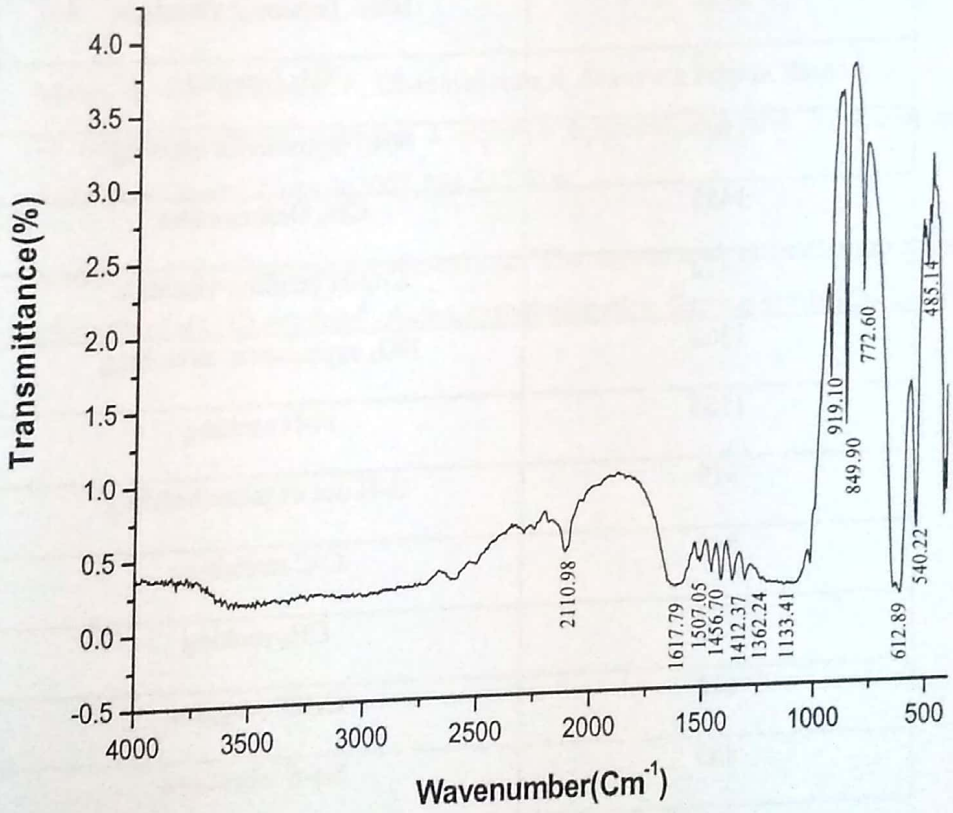

Figure:3. FTIR spectra of Sodium sulphate doped L-Alanine crystal

The N-H asymmetric stretching occurs at 3567 cm^{-1}. The peak at 2110 cm^{-1} is due to NH_3^+ torsional vibration. NH_2 bending is due to a peak at 1617 cm^{-1}. The peaks at 1507 cm^{-1} is due to NH_3^+ symmetric bending. The CH_3 degenerative deformation occurs at 1455 cm^{-1}. The peaks at 1412 cm^{-1} is due to C-O-C bending vibration. NO_3 asymmetric stretch is a peak at 1362 cm^{-1}. The peak at 1133 cm^{-1} is due to N-N rocking. O-H out of plane bending is a peak at 919 cm^{-1}. The peak at 849 cm^{-1} is due to C-C stretching. CH_2 rocking occurs at 772 cm^{-1}. The peak at 612 cm^{-1} is due to COO^- wagging. COO^- deformation occurs at 540 cm^{-1}. The peak at 485 cm^{-1} is due to Na-S vibration. Frequencies and the corresponding assignments are given in table 1.

Table 1.The Frequency Spectral Assignment for Sodium sulphate doped L-Alanine

Wavenumber (cm^{-1})	Assignment
3567	N-H asymmetric stretching
2110	NH_3^+ Torsional vibration
1617	NH_2 bending
1507	NH_3^+ Symmetric bending
1455	CH_3 Deformation
1412	C-O-H bending vibration
1362	NO_3 asymmetric stretching
1133	N-N rocking
919	O-H out of plane bending
849	C-C stretching
772	CH_2 rocking
612	COO^- wagging
485	Na-S vibrations

4. Conclusion

Single crystal of sodium sulphate doped L-Alanine crystal was grown by slow evaporation method. X-ray diffraction studies were carried out and the lattice parameters are

evaluated. The result showed the crystal belongs to orthorhombic system. FTIR studies revealed the presence of various functional groups in the crystal.

5. References

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