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Optical behavior of L-Serine Phosphate, a Semi-organic improved NLO Single Crystal

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Abstract:

Nonlinear optical activity of single crystal of semi- organic amino acid L-Serine Posphate was developed by simple slow evaporation technique. Solubility study of the prepared compound was measured and metastable zone width was found. Single crystal X-ray diffraction (XRD) study was carried out for the grown crystal. The optical properties of the crystal were confirmed by UV-Vis analysis and powder SHG tester. The Fourier Transform-Infrared Spectroscopy (FT-IR) study fairly agrees with the XRD results and functional groups were analyzed. Vickers' micro hardness studies proven the mechanical strength of the grown crystal.

Keywords: L-Serine Posphate ,single crystal, Linear and Non-Linear, strength

I. Introduction

The Importance of nonlinear optical crystals in science and technology has been recognized recently for numerous important applications [1, 2]. This includes sensors, waveguide, transmission, infrared detectors, polarizer, transducers, and for image processing. Due to the efficacy in generating new frequencies from existing laser via harmonic generation, tremendous efforts have been made to identify new materials for such process. Organic and semi-organic materials remain the most widely used crystals for frequency conversion. Organic crystals have a large nonlinear coefficient compared to inorganic crystals. But organic crystals are very sensitive to the presence of intrinsic defects and phonon subsystem [3, 4]. Inorganic crystals have high mechanical and thermal stability than that of organic crystals [5, 6]. Semiorganic crystals are those which combine the positive aspects of organic and inorganic materials resulting in desired nonlinear optical properties. Complexes of amino acids with organic and inorganic salts have been identified as promising

materials for producing second harmonic generation (SHG) because of their bonding properties with the ions of organic and inorganic salts. Amino acids are playing vital role in the field of nonlinear optics. L-Serine is one of the amino acid family crystals which are easily available in nature. The molecules of L-serine can combine with anionic, cationic, and overall neutral constituents. The study on growth of L-serine crystals from aqueous solution with hydrochloric acid , sodium fluoride, formic acid , sodium nitrate , and acetic acid is reported in recent years. Orthophosphoric acid is highly polar in nature. It is easily miscible with water. Crystal structure of L-serine phosphate ($C3O3NH7{\cdot}H3PO4$) was reported early. In the present investigation, good optical quality L-serine phosphate (LSP) single crystal has been grown from aqueous solution by slow solvent evaporation method. Single crystal X-ray diffraction study has been carried out to confirm the crystalline nature of the grown crystal. FT-IR, studies were also carried out for the grown crystal.

II. Experimental Method

8 gm of L-Serine substance was taken and dissolved in double ionized distilled water and saturated solution of L-Serine was prepared. The pH value of the saturated solution is 3.7 maintained and it was allowed to evaporate at room temperature by magnetic stirring. Fine quality, extremely transparent crystal of L-Serine was collected in a period of 24 days.

III. Results and Discussions

a. Solubility and Metastable Zone Width Measurement.

The solubility of L-Serine was determined in the temperature range from 30° C to 60°C using water, acetone, and methanol as solvents. Initially, the temperature is fixed as 30°C and the LS salt is added step by step into 100 mL of deionized water and in other two solvents. The solution is stirred continuously till the supersaturation is achieved [7]. From the studies, it is clear that metastable zone width decreases with the increase in temperature. Larger zone width at lower temperature shows that the LS crystal is a suitable material to grow by slow evaporation technique [8].

b. Single crystal X-ray diffraction (XRD) Studies.

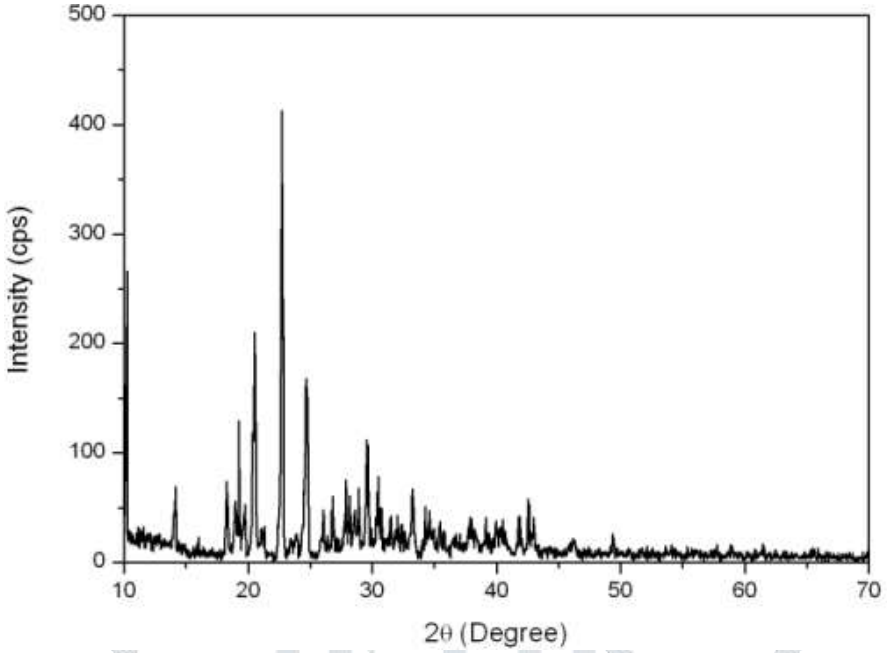

Fig.1 single crystal XRD analysis of L-serine

The grown crystal of L-serine was studied using single crystal XRD analysis to confirm the crystalline nature and also to find the lattice parameters by employing Enraf Nonius CAD 4 single crystal XRD diffractometer with MoKα (0.71073A). From the single XRD data, it is observed ˚ that LS crystallizes in orthorhombic crystal system with the space group $P2_12_12_1$. The lattice parameter values are in good agreement with the data reported earlier [9,10].

Table : 1 Lattice parameters of L-serine

Axial length (Å)	**L-serine**	**Reported value (Å)**
a (Å)	8.532	8.508
b (Å)	9.13	9.12
c (Å)	5.527	5.321
Volume ($Å^3$)	430.47	438.21

c. The Fourier Transform-Infrared Spectroscopy (FT-IR)

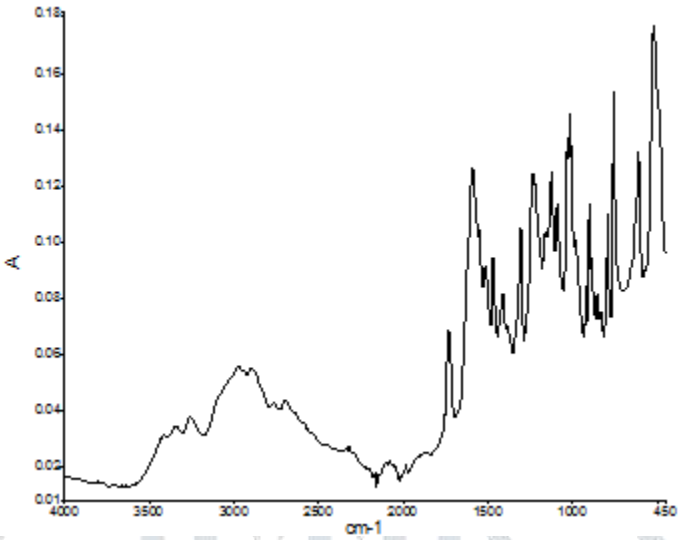

Fig2: The Fourier Transform-Infrared Spectroscopy (FT-IR) analysis of L-serine

The Fourier Transform-Infrared Spectroscopy (FT-IR) analysis was done for the grown LS crystal to find the functional groups of the prepared crystal. A fine powdered sample of LS was used for the FT-IR spectral analysis and the spectrum was recorded in the range 450 cm^{-1}– 4000 cm^{-1} using KBr pellet technique. The peak at 3091 cm^{-1} is an indication of the presence of NH^{3+} groups in the crystal. The peaks at 2733 cm^{-1} and 2566 cm^{-1} are attributed to the C–H stretching mode vibration [11,12]. The CO O^{-} symmetric stretching vibration modes are confirmed at the peaks 1402 cm^{-1}, 1336 cm^{-1}, and 1371 cm^{-1}. Asymmetric deformation of NH^{3+} is confirmed by the peak at 1597 cm^{-1}. The strong absorption peak at 1630 cm^{-1} indicates the presence of primary amino acid group[13]. The multiple combination and overtone bands extended the absorption of hydrogen bonded N–H stretching vibration to 2000 cm^{-1}.

IV. Conclusions

Single crystal of L-Serine was successfully grown by slow evaporation technique and the cell parameters of the crystal confirmed by various characterization techniques. From the Single crystal XRD studies that LS crystallizes is a orthorhombic crystal system. Solubility study and metastable zone width of the crystal have been found. Linear optical studies show the transparency of the crystal in the visible region. FT-IR spectrum of the crystal elucidates the presence of various functional groups in the crystal.

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