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Structural, Linear and Nonlinear Optical Properties of L-Serine Single Crystal

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Abstract: - Nonlinear optical (NLO) materials, with high frequency conversion efficiency have the most applications in the areas such as optical communication and optical storage devices. Amino acids family crystals possess high NLO efficiency because of their non- centrosymmetric space group and chiral carbon atom. L-Serine is an organic amino acid and exists in zwitterionic form. Organic amino acids L-serine was grown by slow evaporation method. The grown crystals have been subjected to single and powder X-ray diffraction, FTIR, UV-visible and Non linear optical studies. The L-Serine was harvested after a period of 20 days. The crystal structure of L-Serine $C_3H_7N0_3$ has been determined by X-ray diffraction methods. It crystallizes in orthorhombic crystal system with space group $P2_12_12_1$ with unit-cell dimensions of a=8.599, b=9.348, c=5.618. FTIR spectrum was recorded and functional groups were analyzed. The linear and non-linear optical properties of the crystal were confirmed by UV-Vis analysis and powder SHG test.

Keywords**:** Organic crystals, X-ray diffraction, FTIR analysis, UV-visible and Nonlinear Optical properties.

I. INTRODUCTION

Nonlinear optical (NLO) materials are having potential applications in the area of telecommunication and optical storage devices. Organic materials are attractive due to their nonlinearities ultra fast response and high laser damage threshold. The zwitterionic forms is important to gain insight into protein folding which is governed by hydrophilic and hydrophobic interactions that determine the H-bonding scheme. L-serine is an organic compound under an aminoacid category. Serine (2-amino-3-hydroxypropane carboxylic acid) is one of these compounds. The alcoholic OH group can act both as proton donor and proton acceptor in hydrogen bonds. Naturally occurring aminoacids have a large conformational flexibility and computational studies should correctly determine conformers and statistical populations found in the experimental data. Crystals of serine are especially interesting in this respect, since serine residues are present at most catalytic active sites. L-serine is an organic compound with the formula $C_3H_7NO_3$. The esterification of the carboxyl group of amino acids plays an important role in the synthesis of peptides, especially due to the increased solubility in organic solvents. In addition, X-Ray Diffraction,Fourier Transform InfraRed spectral analysis, UV-Vis absorption spectroscopy analysis and Non-linear opticals have been performed in details.

II. CRYSTAL GROWTH

L-serine was taken and dissolved in double ionized distilled water, and stirred continuously for four hours to prepare homogeneous solution. The prepared solution was filtered using wattman filter paper and the clear filtrate was left undisturbed at room temperature. Slow evaporation of the solvent resulted in the formation of transparent crystals after four weeks which were isolated by filteration, washed with little ice cold water and dried in air to get the crystalline product. The transparent grown crystal is depicted in fig.1.

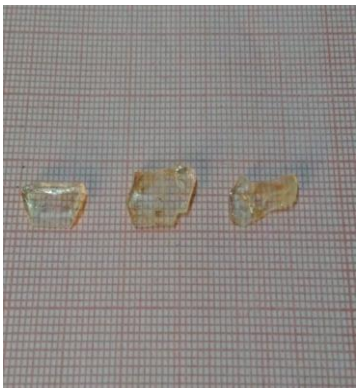

Figure : 1 Grown crystal of LS

III. CHARACTERIZATION

A. X-Ray Diffraction Analysis

The powder XRD studies of pure L-Serine crystals were carried out using an Oxford Diffraction Gemini R Ultra X-Ray diffractometer with a CCD area detector and MOKα (0.71 Å) radiation. From the sharp peaks of XRD pattern indicate high degree of crystalline structure of grown crystal. The observed diffraction pattern has been indexed and miller indices were estimated by Joint Committee on Powder Diffraction Standards (JCPDS) software packages.

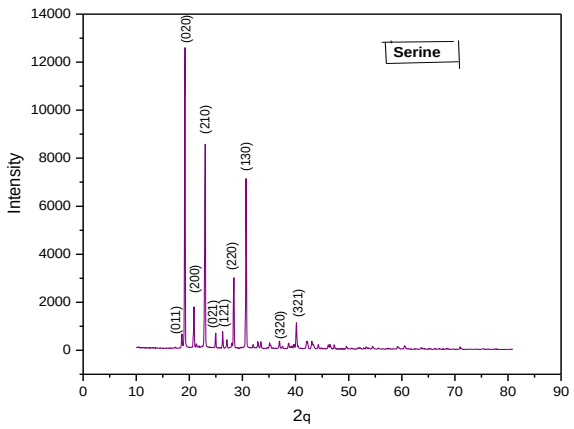

Figure 2: XRD Pattern of Grown crystal.

The observed Powder XRD pattern, the crystallographic data and the lattice parameter values for L-Serine crystals are given in the fig.2 and table 1.

B. Fourier Transform Infrared Spectroscopic Analysis

The FTIR spectrum identifies the functional groups in the region of frequency 400-4000 cm^{-1} by the KBr Pellet technique. The absorption band at 3462 cm^{-1} and 3091 cm^{-1} are assigned to OH Stretching Vibrations and NH_3^+ groups are present respectively. The C-H Stretching is observed at 2920 cm^{-1}. The peak at 2741cm^{-1} e is due to the C-H Stretching mode vibration. The 2000 cm^{-1} are observered at N-H Stretching vibration. The COO^- Symmetric stretching vibration modes are confirmed at the peaks 1410cm^{-1}. The CH_2 bending Vibrations are due to 1381 cm^{-1}. The 1124 cm^{-1} and 609cm^{-1} shows the bands at C-OH and COO^- rocking respectively. These values are found to be in good agreement with the reported values of L-Serine. The FTIR spectrum and the complete assignments to the vibrational frequencies of L-Serine crystal are provided in the fig.3.

Table 1: Cell parameter values

Parameters	L-Serine
Chemical formula	$C_3H_7NO_3$
Crystal System	Orthorhombic
Space group	$P2_12_12_1$
a (Å)	8.599Å
b (Å)	9.348Å
c (Å)	5.618Å
v ($Å^3$)	451.59Å
$\alpha = \beta = \gamma$	90°

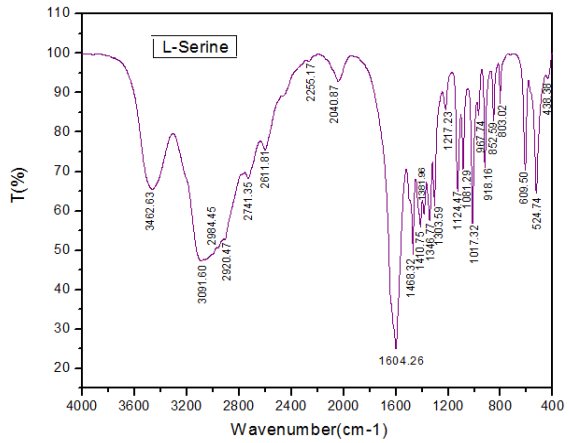

Figure 3: FTIR spectrum of grown crystal

C. UV-Visible spectroscopic Analysis

The optical transmission spectrum of L-Serine crystals were recorded by UV-Visible spectrophotometer in the range 200nm-1100nm.

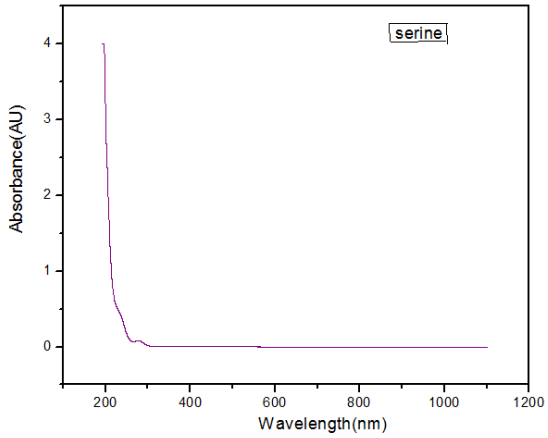

Figure 4: Transmittance spectrum of grown crystal

From the spectrum, it is clear that the LS crystal is highly transparent in the entire visible region with the lower cut off wavelength of 208nm. The UV-VIS transmittance spectrum and absorption spectrum of grown sample is presented in fig. 4 and 5.

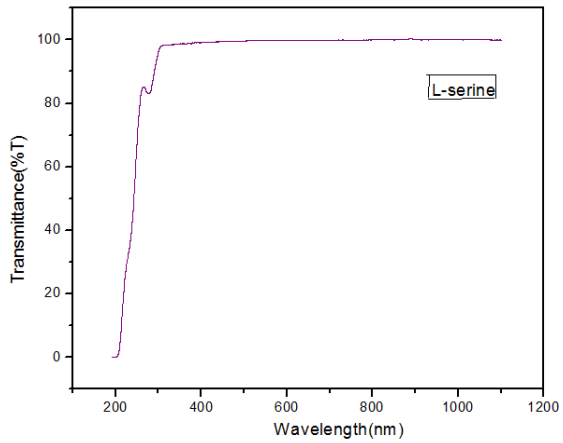

Figure 5: Absorption spectrum of grown crystal

The optical absorption co-efficient (α) is calculated using the following relation,

Where T is the transmittance and d is the thickness of the crystal. The energy dependence of absorption coefficient suggests the occurrence of direct band gap and hence it obeys the relation for high photon energy.

$$\alpha h\nu = A\,(h\nu - E_g)^{1/2}$$

Where, α is the absorption coefficient, E_g is the optical band gap energy, hν is the incident photon energy and A is a constant dependent on electron and hole effective masses. The variation of (hν) vs $(\alpha h\nu)^2$ is shown in figure.6 and E_g value is evaluated by extrapolation of the linear part to a point $(\alpha h\nu)^2 = 0$.

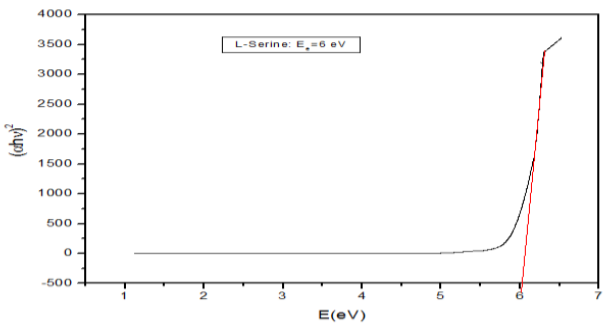

Fig 6:Tauc's plot for grown crystal

The optical bandgap is found to be 6 eV for single L-Serine respectively. As a consequence of wide band gap, the grown crystals have large transmittance in the visible region which enables these materials for higher harmonic generation.

D. Nonlinear optical Studies

The Nonlinear optical conversion efficiency has been carried out using Kurtz and perry powder technique. It is an important and a popular tool to evaluate conversion efficiency of NLO materials. It enables to measure the SHG efficiency of new materials relative to standard potassium dihydrogen phosphate (KDP). A Q-Switched ND:YAG laser operating at the fundamental wavelength of 1064 nm, generating an input power of 30mJ/pulse was used for the present study. The Second harmonic signal generated in the crystalline sample was confirmed from the emission of green radiation of wavelength 532 nm from the crystalline powder. The SHG output was converted into electrical signal and was displayed on a digital storage oscilloscope. The output signal of 46mv for LS crystal was obtained for an input of 30mJ/pulse compared with the SHG output signal of standard KDP crystal of 55mv for the same input energy. From the obtained data, it is found that SHG efficiency of the grown LS crystal is 0.84 times that of KDP crystal.In addition to identifying the materials with non-centrosymmetric crystal structures, it is also used as a screening technique to identify the materials with the capability for phase matching. The continuous increase of SHG with increase of particle size confirms the phase matching behavior of the material. Only those materials exhibiting a phase matching behavior are grown into single crystals of large size for NLO applications.

CONCLUSION

L-serine organic single crystals have been grown by slow evaporation solution growth technique. The powder XRD studies for the grown crystals have been carried out and it is found that the L-Serine crystal crystallizes in orthorhombic crystal system with the space group of $P2_12_12_1$. The unit cell parameter of the L-Serine crystal obtained from the XRD studies are a=8.599 Å, b=9.348Å, c=5.618 Å and V=451.59 $Å^3$. The various functional groups of the grown L-Serine crystals such as OH Stretching Vibration, NH_3^+ group, C-H Stretching, C-H Stretching mode Vibration, N-H Stretching Vibration, COO^- Symmetric Stretching Vibration, CH_2 bending Vibration, C-OH rocking, COO^- rocking have been identified from FTIR spectra. The optical studies show the transparency of the crystal in the entire visible region with a UV cut-off wavelength of 208 nm. SHG studies confirm the nonlinearity of the grown crystal by the emission of green light and the SHG efficiency of the grown LS crystal is found to be 0.84 times that of KDP crystal. Owing to the wide optical transparency and relatively high SHG efficiency L-Seine crystals are the potential candidates for laser applications and fabrication of optoelectronic devices.

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