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STRUCTURAL, OPTICAL, MECHANICAL STUDIES ON TGZC CRYSTAL

[1] M. Akilan, [1] R. Ragu, [1] J. P. Angelena, [1] J. Mary Linet, [1] S. Jerome Das
[1] Department of Physics, Loyola College, Chennai, India 600 034.

ABSTRACT- The development of highly effective NLO materials has been the main focus of current researchers owing to its importance in providing the key functions of frequency shifting, optical modulation, optical switching, optical memory for the emerging technologies in various areas of applied technology such as telecommunications, signal processing, optical interconnections. Tris Glycine Zinc Chloride (TGZC) single crystals were grown successfully by slow evaporation method at ambient temperature. X-ray Diffraction analysis (XRD) was used to estimate the cell parameters of the solution grown TGZC crystal. The presence of various functional groups and its modes of vibration were attained from FTIR spectral analysis. UV study shows no significant absorption in the region 300-800nm and it is found that the crystal has the lower cut-off wavelength about 250nm. The mechanical properties of the grown TGZC crystal are estimated.

Keywords- [Slow evaporation technique, X-ray Diffraction, FT-IR, Optical, Microhardness]

1. INTRODUCTION

Non linear optical (NLO) materials are the key materials which play a predominant role in the recent developments of laser science and technology. Recently number of researchers emphasis on the hunt of semi-organic NLO materials for several applications in frequency conversion, optical data storage, optical switching and electro-optical modulation [1-3]. Glycine is a simplest amino acid and it forms number of complexes with various inorganic salts [4]. Amino acid family crystals have been subjected to extensive investigation over the years by several researchers for their non-linear optical properties [5]. Some complexes of glycine with HCl [6], lithium sulfate [7], $LiNO_3$ [8], sodium nitrate [9] form single crystals, but some of these are reported to have NLO property and some are reported not to have NLO property. In this present work, Tris Glycine Zinc Chloride has been grown by slow evaporation method and have achieved good quality crystal and the systematic investigations has been carried out on grown TGZC crystal such as XRD, FTIR, UV, Microhardness and Dielectric studies.

2. MATERIAL SYNTHESIS

Commercially available glycine and zinc chloride were taken in molar ratio 3:1 and the mixture is dissolved using triple-distilled

water in a growth vessel and kept for slow evaporation in dustproof condition. The following reaction is given below

$3C_2H_5NO_2+ZnCl_2 \rightarrow (C_2H_5NO_2)_3ZnCl_2$

The attempt was successful by obtaining colorless, transparent and good quality single crystal of size 15× 13 x 3 mm^3 was obtained in a period of three weeks and the photograph of as-grown crystal is shown in fig 1.

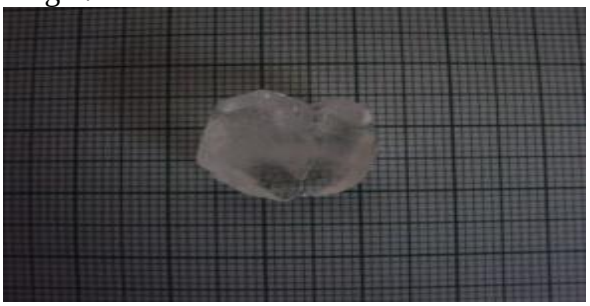

Figure 1- Photograph of as grown TGZC crystsl

3. RESULTS AND DISCUSSION

3.1. Single crystal X-ray diffraction analysis

The single crystal XRD analysis has been carried out using ENRAF NONIUS CAD4 diffract meter with MoKα radiation (λ=0.7170 Å) to determine the unit cell dimensions of the grown crystal. The XRD result shows that the grown crystal belongs to orthorhombic system with space group $P_{bn}2_1$ and the lattice parameters are a = 11.3058 Å, b = 15.2012 Å, c = 15.5520 Å, α=β=γ= 90^0 and V= 2650.69$Å^3$.

3.2. FTIR analysis

The infrared spectral analysis was carried out to understand about the chemical bonding and molecular structure of the compound. The FTIR spectrum of TGZC crystal was recorded in KBr phase in the frequency region 450-4000 cm^{-1} using PERKIN ELMER SPECTROMETER. The broad peak at 1638 cm^{-1} corresponds to C=O group. The peak arises at 1606 cm^{-1} is due to NH_2 deformation and the existence of amino acid confirms that it is COO^- stretching. The very broad peak at 3186 cm^{-1} corresponds to O – H stretching. The spectral assignments of TGZC crystal is shown in Table 1.

Wave number (cm^{-1})	Tentative Assignment
1606	COO^- stretch
1638	C = O stretch
3186	O-H stretch
1126	C-N stretch
2963	CH_2 symmetry and anti-symmetry stretch

Table 1- Spectral assignments of TGZC crystal

3.3. UV-Vis Spectroscopy

The optical transmittance was recorded using sample of thickness 1 mm in the wavelength range from 200 – 800 nm using VARIAN CARY 5E UV-Vis-NIR spectrometer. There is no significant absorption in the range 300-800 nm and it is found that the crystal has the cut-off wavelength about 250 nm. The crystal can be used for NLO applications.

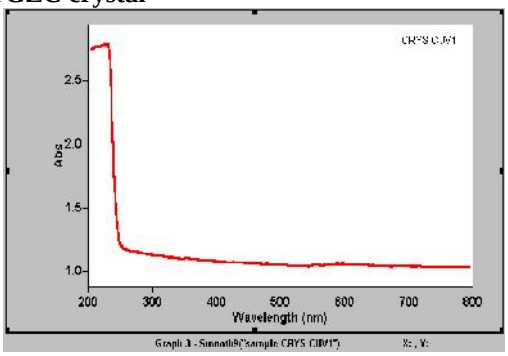

Figure 2- UV visible spectrum of TGZC crystal

3.4. Vickers Microhardness study

The mechanical strength of the grown crystal was done using the instrument Futuretech FM-800 type E series hardness tester. The hardness of crystal provides detail about the strength, molecular bindings and the resistance that the lattice offers to the local deformation. The diagonal length of indentation for applied load P (g) between 25 g to 100 g using Vickers diamond pyramidal indenter, H_v is calculated using the relation

$$H_v = 1.8544\ P/d^2 \quad (1)$$

Where P is the applied load in g, d is the diagonal length in mm and H_v in kg/mm^2. The variation of H_v with the applied load of TGZC crystal as shown in fig 3. The plot of log P vs log d is shown in fig 4 and it yields a straight line and the slope gives work hardening coefficient 'n'. The value of n is 3.75 and it is more than 2 so it is soft material. (Onitsch 1947)

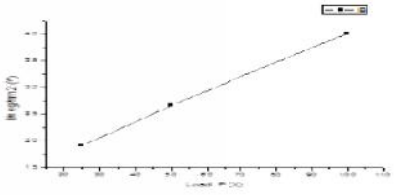

Figure 3- Variation of load P Vs H_v

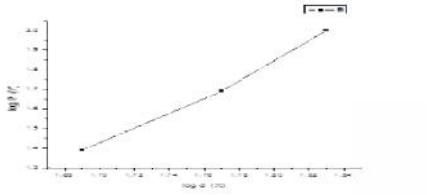

Figure 4- Variation of log d Vs log P

CONCLUSION

TGZC has been grown by slow evaporation technique and have achieved good quality crystal. The single crystal X-ray diffraction analysis depicts that the grown crystal belongs to orthorhombic system with space group $P_{bn}2_1$. The presence of functional groups is confirmed by FTIR spectroscopy. UV spectrum shows that the lower cutoff wavelength is around 250 nm. The microhardness study reveals that the grown crystal is belong to soft material category.

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