International Journal of Technical Research and Applications e-ISSN: 2320-8163,
www.ijtra.com Special Issue 37 (February, 2016), PP. 83-85

GROWTH, STRUCTURE AND FUNCTIONAL PROPERTIES OF ZINC CHLORIDE DOPED L-PHENYLALANINE PERCHLORATE

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Abstract— **Single crystals of Zinc chloride doped L-Phenylalanine Perchlorate were synthesized and grown by slow evaporation method at room temperature. Single crystal XRD data reveal that the crystal belongs to triclinic system. The doping of zinc chloride into the L-Phenylalanine Perchlorate was confirmed using EDAX spectral study. The presences of functional groups were identified using FTIR study. The optical characterization has been done by UV –Vis - NIR spectral studies. Dielectric constant and dielectric loss measurements were carried out at different temperatures and frequencies to analyse the dielectric behaviour of the grown material required for induced polarization.**

I. INTRODUCTION

Recent advancement in the field of science and technology has pushed mankind to tailor new NLO materials. In view of developing a new NLO material, Zwitterionic natured amino acid was found to be a suitable material for growing amino acid complexes with enhanced NLO activity. Here L-Phenyl alanine perchloric acid was chosen as it is used in the treatment of neurotransmitters [1-4]. The metal dopant Zinc chloride was considered due to its high electrical conductivity. The combination of Zinc chloride doped L-Phenylalanine perchlorate is expected to possess both NLO and electrical property which finds applications in optical, electrical and photonic industries. In the present study, bulk single crystals of Zinc chloride doped L –Phenylalanine perchlorate has been grown by slow evaporation technique. The grown crystals were subjected to single crystal XRD, EDAX, FTIR, UV – Vis – NIR and dielectric studies.

II. EXPERIMENTAL

L-Phenylalanine, Perchloric acid and Zinc chloride were used to synthesize Zinc chloride doped L-Phenylalanine perchlorate single crystals. The starting materials were taken withmolar ratio 2:1:1. The calculated amounts of L-Phenylalanine, Perchloric acid, Zinc chloride were dissolved in mixed solvent of deionized water and HCl. The solution was stirred well using magnetic stirrer, filtered and kept for slow evaporation. Transparent crystals of size 28 × 5 × 4 mm^3 were obtained. Fig. 1 shows the picture of the as - grown zinc chloride doped L-Phenylalanine perchlorate crystal.

Fig 1. Photograph of the Zinc chloride doped L-Phenylalanine perchlorate crystal.

III. SINGLE CRYSTAL XRD

KAPPA AEX – II single crystal diffractometerwas used to analyse the single crystal X-ray diffraction. Single crystal XRD data reveal that the crystal belongs to triclinic system withspace group P_1. The cell parameters were found to be a = 5.13 Å, b = 13.55 Å, c = 26.53 Å and α = 85.70°, β = 87.88°, γ = 89.98° and V = 1839 $Å^3$.

IV. EDAX

The presence of different components of the synthesized material was confirmed by EDAX analysis as shown in Fig. 2. The presence of various elements carbon, nitrogen, oxygen, zinc and chlorine has been confirmed by the respective peaks in the spectrum. Table 1 shows the presence of various elements with atomic and weight percentage.

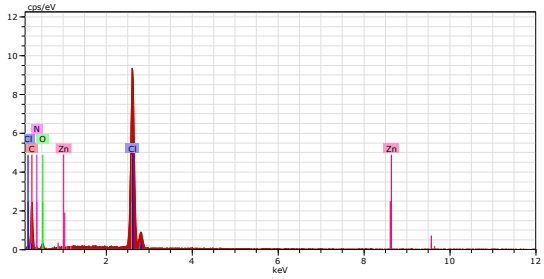

Fig 2. EDAX analysis of Zinc chloride doped L-Phenylalanine Perchlorate single crystal

Element	Weight %	Atomic %

C	65.92	76.28
N	9019	9.12
O	10.21	8.87
Cl	14.57	5.17
Zn	0.11	0.02

Table 1.Composition of Zinc chloride doped L-Phenylalanine Perchlorate single crystal

V. FTIR SPECTRAL ANALYSIS

FTIR spectrum of the grown Zinc doped L-Phenylalanine perchlorate single crystal was recorded in the range of 4000 cm^{-1}– 400cm^{-1}using the FTIR spectrometer. The FTIR spectrum of Zinc doped L-Phenylalanine a perchlorate single crystal is shownin Fig. 3. The various frequency assignments of the grown crystal are shown in Table 2. The presence of $N^{+}H_3$ and COO^- is understood from the table [1, 2].

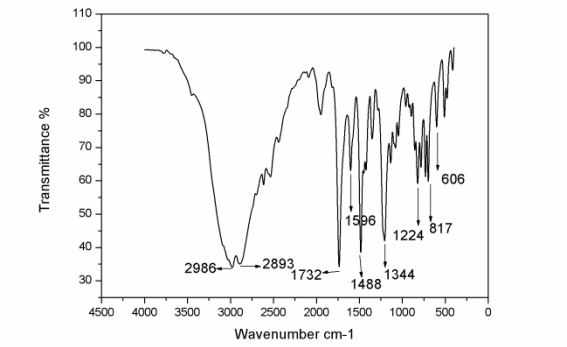

Fig 3. FTIR spectrum of Zinc chloride doped L-Phenylalanine Perchlorate single crystal

Wavenumber (cm^{-1})	Assignments
2986 and 2893	C – H stretching
1732	COO^- stretching
1596	$N^{+}H_3$ symmetric bending
1488	CH deformation
1344	C – H deformation
1224	COO^- stretching
817	C – H bending (para)
602	ClO^2 rocking; Phenyl ring in plane deformation

Table 2 FTIR frequency assignments of Zinc chloride doped L-Phenylalanine Perchlorate single crystal

VI. UV – VIS – NIR OPTICAL ABSORPTION SPECTRUM

UV – vis – NIR optical absorption spectrum was carried out in the range of 190 nm - 1100 nm for Zinc doped L-Phenylalanine perchlorate crystals. Fig. 4 shows the absorption spectrum of the grown crystal is found to possess wide transmission range in the region of 190 – 1100 nm with lower cut off wavelength at 302 nm. Fig. 5shows the plot of $(\alpha h\nu)^2$against hν. From the plot, the optical band gap was estimated as 3.86 eV. The higher band gap value indicates the dielectric behaviour of the material.

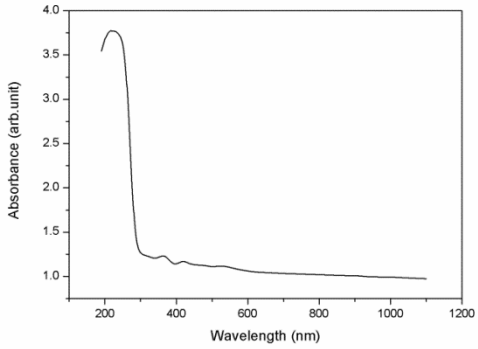

Fig 4. UV – vis – NIR absorbtion spectrum of Zinc chloride doped L-Phenylalanine Perchlorate crystal

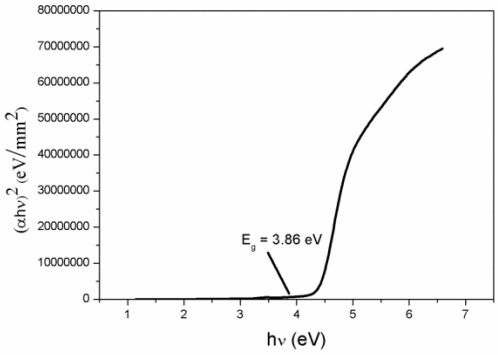

Fig 5. Plot of $(\alpha h\nu)^2$vs photon energy (hν) for Zinc chloride doped L-Phenylalanine Perchlorate crystal

VII. DIELECTRIC STUDIES

Dielectric studies were carried out for the grown material at different temperatures for various frequencies. The variation of dielectric constant with frequency at different temperatures for Zinc chloride doped L –Phenylalanine Perchloric acid single crystal are shown in Fig. 6. The decrease of dielectric constant with frequency shows the dependence of dielectric constant on electronic, ionic and space charge polarization. Fig. 7 shows the variation of dielectric loss with frequency. From the variation of dielectric constant and dielectric loss with frequency, the dielectric behaviour of the grown material is understood.

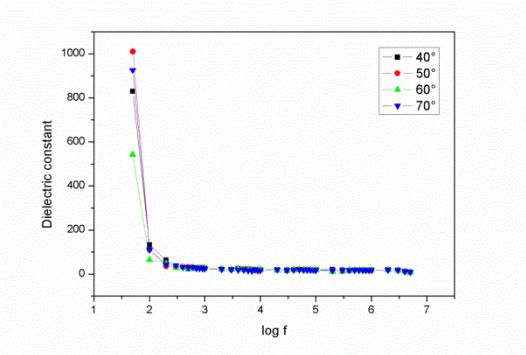

Fig 6. Plot of log f vs dielectric constant for Zinc chloride doped L-Phenylalanine Perchlorate crystal

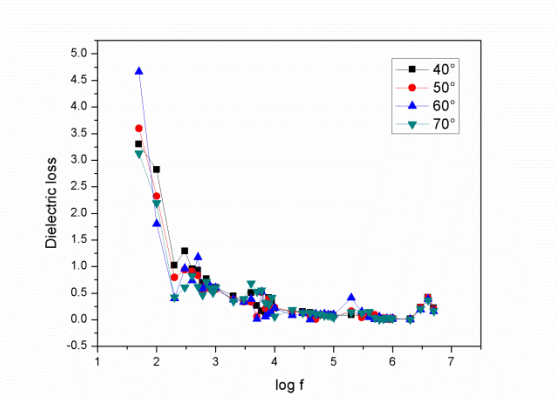

Fig 7. Plot of log f vs dielectric loss for Zinc chloride doped L-Phenylalanine Perchlorate crystal

VIII. Conclusion

Zinc chloride doped L-Phenylalanine Perchlorate crystals were grown using slow evaporation technique. Single crystal XRD results show that the grown crystal is triclinic with space group P_1. EDAX analysis confirms the presence of the elements zinc, chlorine, carbon, nitrogen and oxygen. The functional groups were identified using FTIR spectrum. The transmission range was measured with the help of UV – vis – NIR optical absorption spectrum. The optical band gap was estimated from Tauc's plot. The dielectric behaviour of the doped crystal was understood from the dielectric study. The dielectric property is essential for any NLO material.

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