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Synthesis, Growth and Characterization of pure and magnesium doped triglycine zinc chloride single crystals

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Abstract: A semi organic crystal triglycine zinc chloride and magnesium doped triglycine zinc chloride were grown by solvent evaporation method. The pure and doped TGZC single crystals were subjected to structural and optical analysis. From the powder XRD studies it was found that TGZC and magnesium doped TGZC belong to orthorhombic crystal structure with $Pbn2_1$ space group**.** It is seen that both pure and doped TGZC are transparent over the entire range of UV- Visible region and the cut off was found to be 228nm. With the increase in the doped percentage from 0.1 to 0.3 there is a decrease in the absorbance which shows that there is an increase in the transmittance. Thus addition of magnesium has increased the transmittance of the TGZC which is very essential for a good NLO crystal. The presence of functional groups and the metal to ligand bonding are identified using FTIR spectrum.
Keywords: Triglycine zinc chloride, XRD, FTIR, UV, NLO.

Introduction and Experimental

The combination of amino acids with inorganic salt has led to the invention of many promising materials for second harmonic generation applications. In amino acid, the carboxylic acid group donates its proton to the amino group to form a salt of structure $NH_3^+CH_2COO^-$ Due to this dipolar nature, amino acids have physical property, which makes them suitable candidates for NLO applications [1]. The tetrahedral in both structures differ only in position of Cl^- ions only *trans* for $2Gly.ZnCl_2.2H_2O$ and *cis* for $3Gly.ZnCl_2$. The Gly zwitterions are monodentately coordinated to Zn^+ ion by one oxygen atom from carboxyl group [2]. Dielectric constant is found to be maximum at 100Hz frequency [3]. The starting materials of analytical grade were used. Glycine and zinc chloride were taken in the ratio 3:1 and were kept for stirring for 6 hours to ensure that the triglycine zinc chloride is formed and some other secondary phases are not formed. The chemical reaction involving the synthesis is as follows.

$$3(NH_2\text{-}CH_2\text{-}COOH) + ZnCl_2 \rightarrow (NH_3\text{-}CH_2\text{-}COO)_3 ZnCl_2$$

After 6 hours of stirring, the white precipitate of TGZC was obtained. The synthesized material was then filtered, dried and recrystallised with water as solvent. After a growth period of 25 days bulk crystal of size 2.5x1.6x1.1cm^3 was harvested. The as grown crystal is shown in the figure 1. 300 ml of saturated solution of 0.1%, 0.2% and 0.3% magnesium doped TGZC were prepared, filtered using Whatman No.1 filter paper. The solutions were then kept at constant temperature bath at 36^{o}C. After a growth period of 30 days bulk crystals of dimensions 1.8x1.1x1xcm^3 (0.1%), 1.8x1x0.5cm3 (0.2%) and1.9x1.2x0.6cm3 (0.3%) was harvested.

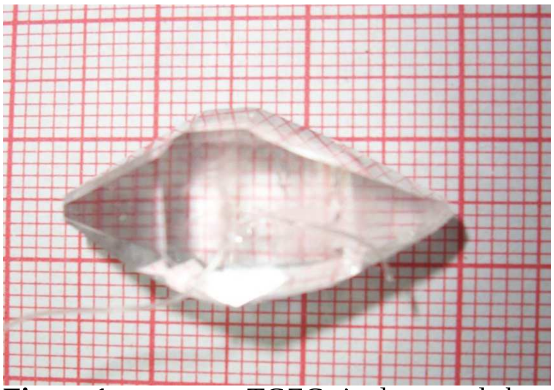

Figure 1: as grown TGZC single crystals by solvent evaporation method

Results and Discussion

Powder X-Ray Diffraction Analysis: The crystalline quality was confirmed by powder X-ray diffraction analysis. The finely crushed powder sample of TGZC was subjected to high intense X-rays of wavelength 1.5418Å (CuKα) at a scan speed of 1°/minute. The powder diffraction pattern corresponding to TGZC and magnesium doped TGZC (0.1%, 0.2%,0.3%) are as shown in Figure 2.Glycine with ZnCl2 crystallizes in the orthorhombic system in the non-Centro symmetric space group Pbn21 [1].

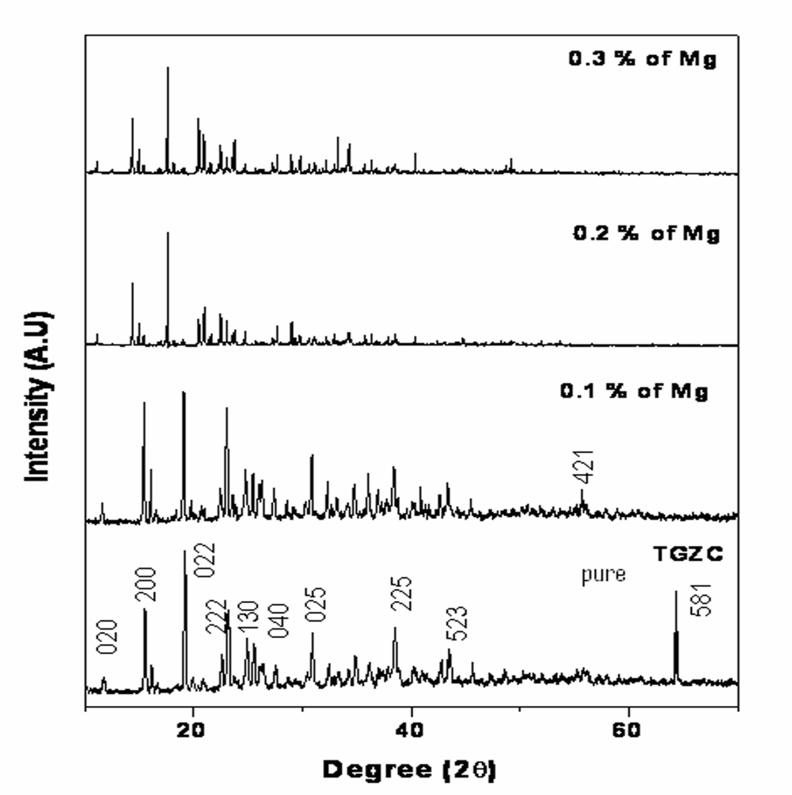

Figure 2: X-ray diffraction pattern

FT-IR Spectral analysis: The FTIR spectrum of the pure and the doped TGZC were studied and the spectrum is shown in figure 3. From the FTIR studies the presence of the functional groups like NH_2, COO^-, CH_2 and the metal to ligand Zn-O bonding have been proved. The board band between 3300 – 3000 cm-1 is due to NH stretching vibration [4] NH symmetric and asymmetric broad single band is observed and assigned to NH vibration. There is a marginal blue shift with respect to percentage of the dopants.

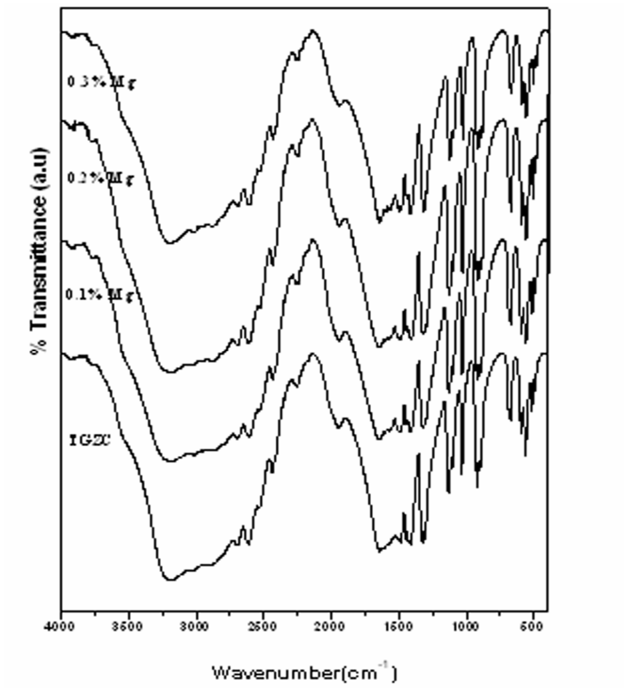

Figure 3: FTIR spectrum of pure and Mg doped TGZC single crystals.

UV-Vis-NIR Spectral analysis: UV region of electromagnetic radiations is 180-400nm and visible region is 400-800nm. Figure 4 shows the absorbance spectrum corresponding to pure and doped triglycine zinc chloride crystals. The absorption spectrum of the crystal is transparent not only in the visible region, also in the near UV region, which is an essential parameter for NLO applications. It is further observed that cut-off of TGZC and doped TGZC is 228 nm and it is suitable for applications in the blue region. As the percentage of doping magnesium increases the absorbance decreases. Thus the doped crystals have lower absorbance than that of the un-doped TG absorption in the visible region is an intrinsic property of all amino acids.

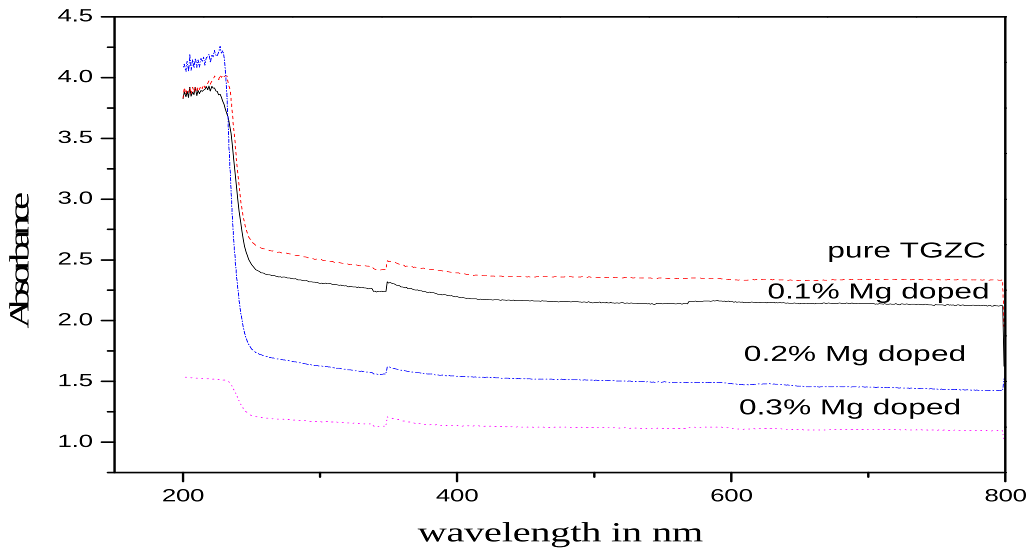

Figure 4: UV – VIS- NIR Spectral

Conclusion

Single crystals of pure TGZC and Mg doped TGZC were grown by slow evaporation technique. Crystal structure analyses by powder X-ray diffraction shows the crystal crystallizes to orthorhombic structure. FT-IR spectroscopy confirmed the functional groups present in the material. UV-Vis spectral studies show the absorbance value 228 nm and increase in magnesium decreases the absorbance.

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