IOSR Journal of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861,
PP 05-08
www.iosrjournals.org

A Study on the Growth and Characterization of a Semi-Organic Non-Linear Optical Glycine Sodium Chloride Single Crystal

K. Jebastin Ganaraj, M. Karthick, P.Ranjith Kumar, M. Shanmuga Raja and N. Boomadevi

Department of Physics, Sri Paramakalyani College, Alwarkurichi, Tirunelveli District, Tamilnadu, India

Abstract: *The single crystal of glycine doped sodium chloride, a semi organic non linear optical material has been grown from solution (pH = 6) by slow evaporation at room temperature. The expected functional groups of the title compound were confirmed by the FTIR spectral analysis. The crystalline nature and its various planes of reflections were observed by the powder XRD. The optical quality of single crystal of glycine doped sodium chloride identified by UV visible studies.*

Keywords: *Glycine, Sodium chloride, FTIR, XRD and crystal.*

I. Introduction

It is thought that development of a new optical device is needed to satisfy the demand in the society. The large non-linear optical properties of large organic molecules and polymers have been the subject of extensive theoretical and experimental investigations during past few decades. Considerable efforts have been made to investigate organic non-linear optical materials. Organic non-linear optical materials are often formed by weak Vander walls and hydrogen bonds and hence possess high degree of delocalization[1]. Nonlinear optical (NLO) materials have long been known to interact with light, to produce a nonlinear response and the composition of these materials, generally falls into three classes, either inorganic, organic or semi organic. Especially the semi organic non linear optical materials requirements ask for a large difference in dipole moment characterizing the interaction between substituent group and electronic cloud, between the ground and excited states of the molecule organized in a non-centro symmetric structure [2]. Glycine is the simplest of all amino acids in the crystalline form, having three different polymorphs in which the molecules exist in the dipolar form. This dipolar nature exhibits peculiar physical and chemical properties of amino acids making them ideal candidates for use in NLO [3].

In recent years, organo-inorganic hybrid materials have attracted considerable attention. In particular, the inorganic derivatives of protein amino acids are often attributed to symmetric groups without an inversion centre mostly to polar symmetry groups. Their crystals have properties whose symmetry is described by odd - rank tensors such as pyro-electric effect, spontaneous electric polarization, piezoelectric effect, generation of second optical harmonics, etc. Moreover crystals that belong to the eleven antiomorphic point groups, having no mirror reflection planes exhibit optical activity, which is described in terms of the axial generation tensors. While the structures of most amino acids are well defined, the structures of the derivatives of the protein amino acids with inorganic components are not [4]. This paper defines the crystal structure of glycine sodium chloride [GSC]. This has been investigated by the FTIR studies, its crystalline nature is studied by the powder XRD, the transmittance and absorbance of electromagnetic radiation is studied through UV-Visible spectrum.

II. Materials And Methods

2.1 Synthesis and crystal growth

GSC was synthesized from analytic grade of Glycine and Sodium Chloride (Merck) in various ratios and was synthesized by distilled water. The pH of the solution at super saturation is kept at 6.0.The glycine is get from Merck company. The solution stirred up to 3 to 4 hours in a magnetic stirrer to get a homogenous solution. The saturated solution is kept in a undisturbed place. The solution is filtered and transferred to a 100 ml Beaker for crystallization. The crystallization takes place after nucleation is occur. The good quality of seed crystals have been produced. The beaker is kept undisturbed for evaporation. After few days most of the solution is evaporated. It is easy to separate the crystals after the evaporation. .The seeds are harvested after a period of two days. Then the pure samples of seed crystals are taken and characterized. These seed crystals were used for the growth of bulk glycine sodium chloride crystals. It is observed that the grown crystals have glycine and sodium chloride with perfect external morphology. The grown crystals had been subjected into primary

characterization such as XRD, FTIR and UV. The characterization shows the crystal type and structure with the observed values.

III. Results And Discussion

1.1 XRD analysis for GSC:

Powder XRD of the crystals was recorded in order to as certain that the crystal is in γ-phases of glycine. We have recorded the powder XRD pattern using XPERTPRO powder X-ray diffractometer with Cu Kα radiation (1.54060 A) at 30 mA and 40 kV. The sample was scanned in the 2θ values from 10 to 80 at a scan step time of 3.175 sec. Figure 4.1 shows the indexed powder XRD pattern of the glycine crystals grown from a mixture of water and sodium chloride. It is clear that the powder XRD pattern of the crystal remained the same except intensity level of the characteristic peak at 25.3 A as reported in refs. [5-7]. The XRD pattern peaks are also coincided with the JCPDS file PDF#060230 and the structure of γ-glycine sodium chloride crystal is hexagonal.

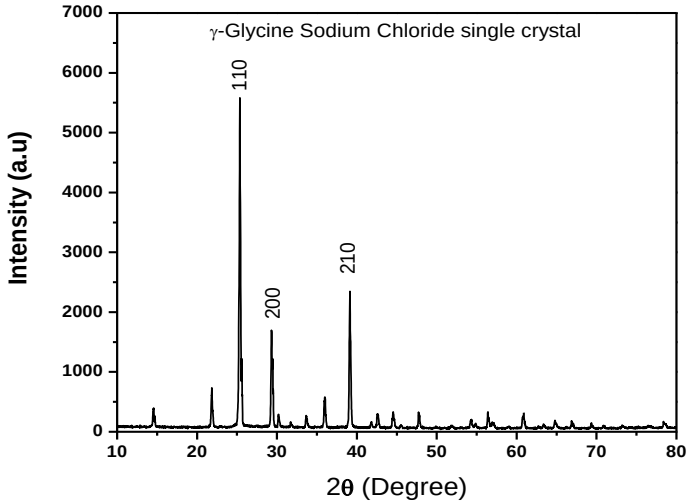

Fig. 1: Powder XRD pattern of γ-glycine sodium chloride single crystal

1.2 UV Analysis Of GSC:

The UV-Vis spectrum of pure and SCG crystals were recorded in the range of 200-800nm using LAMBDA-35 UV-Vis spectrophotometer. The γ-glycine sodium chloride single crystal UV absorption is appeared at 224 nm, 303 nm, 314.5 nm and 341 nm and the absorption is very small. There is no absorption through the entire visible region, that is, the transmission property of the crystal is very high. The UVVis absorption spectrum is shown in fig.4.2. It is one of the most desired properties of non-linear optical material. From the figure 4.3, we have measured the band gap energy E_g = 3.92794872 eV of the GSC crystal.

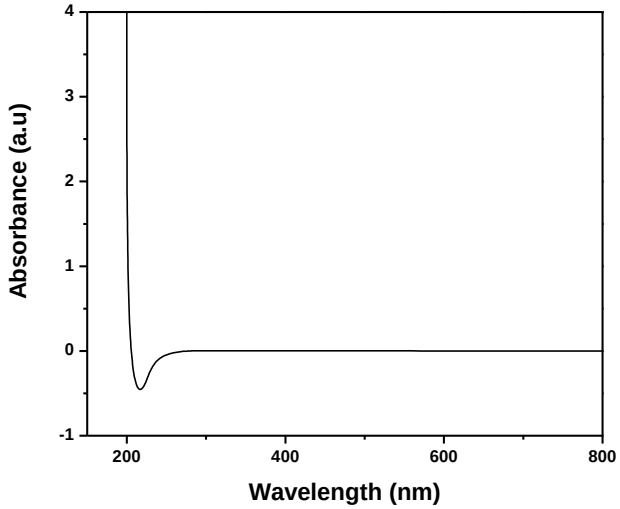

Fig. 2: UV-Vis spectrum of γ-glycine sodium chloride single crystal

The absorption spectroscopy is very useful to calculate the optical band gap (Eg). From the classical relationship of near edge optical absorption of semiconductors,

$$\alpha = k(h\nu - E_g)^{n/2}/h\nu \quad (1)$$

where k is constant, E_g is the optical band gap and is a constant equal to 1 for direct band gap semiconductors. The plot of $(\alpha h\nu)^2$ against hν is shown in Fig.3 and extrapolating the straight line of this plot for zero absorption coefficient.

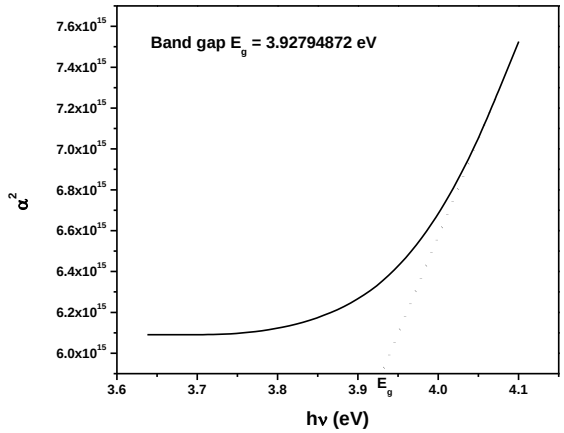

Fig. 3: UV-Vis spectrum of γ-glycine sodium chloride single crystal

1.3 FTIR studies of GSC:

The powdered specimen of sodium choloride doped glycine crystal has been subjected to FTIR analysis by PERKIN ELMER RXI Fourier Transform Infrared Spectrophotometer using KBr pellet technique in the wavelength range between 400 and 4000 cm^{-1} . The recorded spectrum of Sodium chloride doped glycine is shown fig. 4.4. The FTIR spectrum of Sodium chloride doped glycine agrees well with literature [8].

The absorption peaks due to carboxylate group are observed at 503.39, 607.54 and 697.22 cm^{-1} respectively. Similarly the absorption peaks due NH^{3+} groups are observed 910.34, 1032.81, 1412.76 cm^{-1} respectively. The presence of NO_3 group is conformed due to absorption peaks at 892.02 cm^{-1}. Peak at 1032.81, 1331.76 and 1412.76 cm^{-1} are attributed to NCN, COO- and NH_2 groups respectively. Others bands of COO- mode deformation were soon at 697.22, 607.54 and 503.39 cm^{-1} in the spectrum.

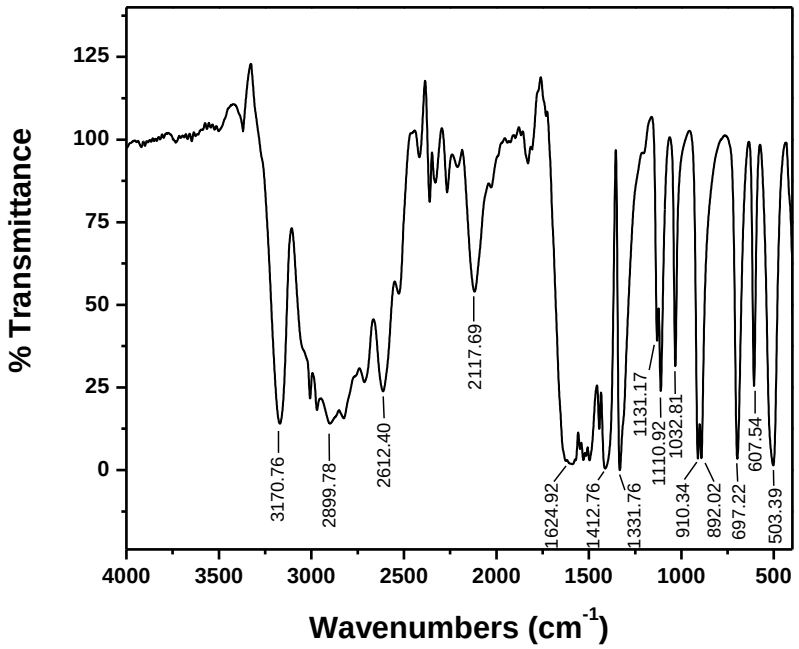

Fig. 4: FTIR Spectrum of γ-glycine sodium chloride single crystal

IV. Conclusion

In the present investigation glycine sodium chloride crystals were grown by slow evaporation method in aqueous media. Transparent crystal shows good morphology with reasonable size. XRD Studies were taken for GSC crystal and the cell parameter were found from the JCPDS file for this XRD data. It shows hexagonal structure. UV absorption studies were done for these peaks to study the band gap energy. The absorption was seen around at 224 nm, 303 nm, 314.5 nm and 341 nm. The band gap energy is 3.92794872 eV. FTIR studies were taken for this sample for conforming functional group present in the material. It shows the presence of NH2 group, COO group and Na+ ions. The absorption peaks due to carboxylate group are observed at 503.39, 607.54 and 697.22 cm-1 respectively. Similarly the absorption peaks due NH^{3+} groups are observed 910.34, 1032.81, 1412.76 cm^{-1} respectively. The presence of NO_3 group is conformed due to absorption peaks at 892.02 cm-1. Peak at 1032.81, 1331.76 and 1412.76 cm-1 are attributed to NCN, COO^- and NH_2 groups respectively. Others bands of COO^- mode deformation were soon at 697.22, 607.54 and 503.39 cm^{-1} in the spectrum.

References

[1] R. Ramesh, M. Aravinthraj, M. Selvam and D. Rajkumar, *Pelagia Research Library Advances in Applied Science Research*, 2 (5), 2011, 136

[2] S. Palaniswamy, O.N. Ranganathan, *Rasayan J.Chem*. 1, 2008, 782

[3] B. Narayana Moolya, S. M. Dharmaprakash, *Mater. Lett.* 61, 2007, 3559

[4] **S**.Palaniswamy and O.N.Balasundara**m,** *Rasayan J. Chem***.** Vol.2(1), 2009, 49

[5] Xia Yang, Jie Lu, Xiu-Juan Wang and Chi-Bun Ching, *Journal of Crystal Growth* 310, 2008, 604

[6] M.N. Bhat, S.M. Dharmaprakash, J. Crystal Growth **242** (2002) 245

[7] B.N. Moolya, A. Jayarama, M.R. Sureshkumar, S.M. Dharmaprakash, *J. Crystal Growth* 280, 2005, 581.

[8] S. Vijayakumar, P. Srinivasan, S. Dinagaran and D. Buvaneshwari, *International journal of chem. tech. research* **6,** 2014, 1673