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Synthesis and Optical Characterization of L-Arginine Doped Gamma Glycine Crystals

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Abstract-- Amino acids play an important role in the field of non linearoptical (NLO) crystals. A amino acid consists of an amino groups, a carboxyl group, a hydrogen atoms and a distinctive R group (side chain), all of which boded to a alpha – carbon. This tetrahedral array of four different groups about alpha –carbon confers optical activity of amino acid. Thus, amino acid is used as dopant in order to enhance the material properties such as nonlinear optical. Based on this , L - arginine, is added with gamma glycine as dopant in various molar percentage. single crystals of glycine lithium chloride was synthesized by solution method and the solubility study was carried out at various temperature ranging from 30-50 oC in aqueous solution. Using the solubility data, saturated solution of the sample was prepared and single crystals of the synthesized salt was grown by slow evaporation method. The study of induction period against supersaturation gives an idea of optimized induction period in order to have a controlled nucleation rate to grow good quality single crystals. Then the grown crystals have been subjected to XRD studies to estimate the crystal structure. The functional groups have been identified by FTIR studies. Ultraviolet-visible (UV-Vis) spectral studies have been carried out.

Keywords-- *NLO, Gamma-glycine*

I. INTRODUCTION

The simplest amino acid 'glycine' is available in many polymeric forms and the gamma-glycine (gamma-glycine) is an asymmetric amino acid that has second-order NLO properties. The gamma-glycine is thermodynamically the most stable form at room temperature but transforms to the gamma-form at high temperatures. solutionThe growth of gamma-form of glycine crystals can be carried out from aqueous solution or gel in the presence of additives, from supersaturated irradiated with plane-polarized laser light [1], or from surfactant based microemulsion and lamellar phases [2]. In this work,gamma-glycine (GG) crystals have been grown using lithium chloride as the additive and to modify the various properties of gamma-glycine, L-alanine and L-arginine were added as dopants. Single crystals of undoped and doped gamma-glycine was grown by solution method with slow evaporation technique at room temperature (31 oC). The grown crystals were characterized to analyze the structural, spectral, mechanical, electrical properties and other properties and the obtained results are presented.

II. MATERIAL SYNTHESIS AND PURIFICATION

Single crystals of gamma-glycine (γ -glycine) was grown by taking AR grade glycine and lithium chloride in 1:1 molar ratio. Initially, the aqueous solution of lithium chloride was prepared in a corning glass beaker and the calculated amount of glycine was added into it. By adding more double distilled water and by stirring using a hot plate magnetic stirrer, saturated solution was prepared and this solution was filtered using high a quality filter paper to remove the unwanted dusts and other particles. Then the filtered solution was allowed for slow evaporation to obtain the crystals. It took about 20 days to get single crystals of gamma-glycine (GG). The sample was re-crystallized again to improve the purity. In this process some good quality crystals was kept inside the saturated solution to obtain big-sized crystals of gamma-glycine. To grow L-arginine doped gamma-glycine crystals, 1 mole%, 2 mole% and 3 mole% of L-arginine were added into the solutions of gamma-glycine and single crystals were obtained by slow evaporation technique.

III. EXPERIMENTAL PROCEDURE

A. Solubility Measurements:

Solubility measurements are an essential pre –requisite for the success of the solution growth technique.For this measurement, a hot plate magnetic stirrer, a digital thermometer and a constant temperature bath (CTB) are necessary. The synthesized salt of glycine lithium Chloride was added in step by step to 50 ml of double distilled water in an air-tight container kept on the hot plate magnetic stirrer maintaining the temperature at 30 oC. After preparing the saturated solution, 5 ml of the solution was pipetted out and taken in a petri dish and it was warmed up at 40o C till the solvent was evaporated out. By measuring the amount of solute present in the petri dish, the solubility of GLS in double distilled water was determined. This method is known as gravimetrical method [3,4]. The same procedure was followed to find solubility of L-arginine doped gamma glycine samples at other temperatures such as 35, 40, 45 and 50 oC Solubility curves for undoped and L-arginine added gamma glycine salts at various temperatures ranging from 30 to 50oC are depicted in the figure 1. As the solubility increases with temperature, the samples have positive temperature coefficient of solubility and hence these samples can be grown in the form of single crystals by slow evaporation method [5,6]

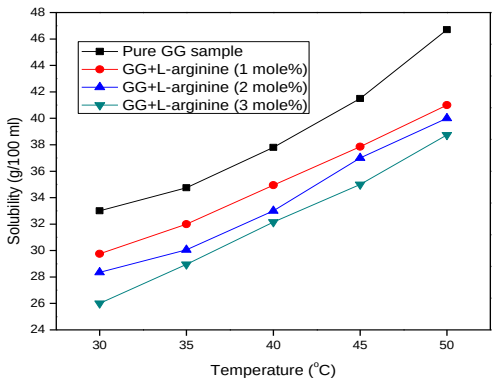

Figure 1: Solubility curves for undoped and L-arginine doped gamma-glycine crystals.

B. Critical nucleation parameters:

Nucleation kinetic studies were performed for the grown crystals of undoped and doped gamma-glycine using a constant temperature bath (CTB). From these studies, the data of critical nucleation parameters were obtained and these data will be useful to understand the nucleation phenomena that are taking place in the supersaturated solutions of samples.The plots of induction period versus supersaturation ratio for undoped gamma-glycine (GG), GG sample doped with L-arginine presented in the figures 2 .

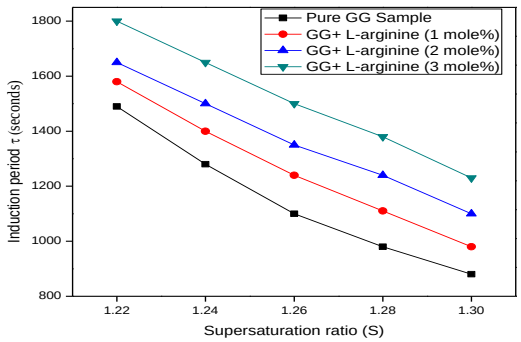

Figure 2: Plots of induction period versus supersaturation ratio for gamma glycinesampledoped with L-arginine

C. XRD studies for identification of crystal structure

Single crystals of undoped and doped gamma-glycine were subjected to single crystal XRD studies using on ENRAF NONIUS CAD4 diffractometer with MoKα radiation (λ = 0.71073 Å) to identify the crystals structure. From the data, it is noticed that all the grown undoped and doped crystals of gamma-glycine crystallize in hexagonal crystal structure. The unit cell dimensions obtained by single crystal XRD studies for the samples are shown in the table 1. The diffraction data shows a very good match with the data reported in the literature [7] .

Table 1: Unit cell constants of undoped and doped gamma-glycine crystals

Crystal	Axial dimensions (Å)	Angular parameters (degrees)	Unit cell volume Å^3
Undoped gamma-glycine (GG)	a= b=7.023 (2) c=5.4780(1)	α=β= 90° γ =120°	234.04
GG crystal doped with 1 mole % of L-arginine	a=b=7.039(4) c=5.486(2)	α=β= 90° γ =120°	235.40
GG crystal doped with 2 mole % of L-arginine	a=b=7.048(1) c=5.490(5)	α=β= 90° γ =120°	236.17
GG crystal doped with 3 mole % of L-arginine	a=b=7.055(4) c=5.496(3)	α=β= 90° γ =120°	236.90

D. Fourier transforms infrared (FTIR) spectroscopic studies:

Functional groups and the molecular structure of compounds can be identified using the infrared spectroscopy. The higher-energy near-IR, approximately 14000–4000 cm−1 can excite overtones and harmonic vibrations. The mid-infrared, approximately 4000–400 cm−1 may be used to study the fundamental vibrations and associated rotational-vibrational structure. The instrument used in this work is a Fourier transform infrared (FTIR) spectrometer and the recorded FTIR spectra of the samples are shown in the figure 3. The assignments for absorption bands of infrared spectra were given in accordance with the data reported in the literature [8,9].

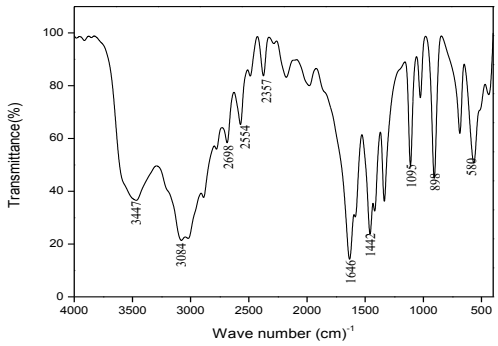

Figure 3: FTIR spectrum of 3 mole% of L-arginine doped gamma-glycine sample

Table 2: FTIR spectral frequencies and their assignments for GG crystal doped with 3 mole% of L-arginine

Wave number (cm)-1	Assignments
3447	NH and OH stretching
3084	NH3+ Stretching
2698	Combination band
2357	Combination band
1646	COO- stretching & NH3+ bending
1442	CH2 bending
1095	C-C-N asymmetric stretching
582	COO rocking

E. Determination of transmittance, optical band gap:

The UV-visible-NIR spectrum gives information about the structure of the molecule because the absorption of UV and visible light involves the promotion of electron in σ and π orbitals from the ground state to higher energy states [10]. The opticaltransmittance spectra of L-arginine doped gamma glycine crystals were recorded using a double beam spectrometer in the 190-1100 nm region and recorded spectra are shown in figures 4. (a), (b) . Optically clear single crystal of thickness about 1.5 mm was used for the transmittance studies. It is observed from the spectra that the sample of gamma glycine doped with 1 mole%, 2 mole% and 3 mole% of L-arginine show the absorption peaks at 397 nm, 395 nm and 390 nm respectively.

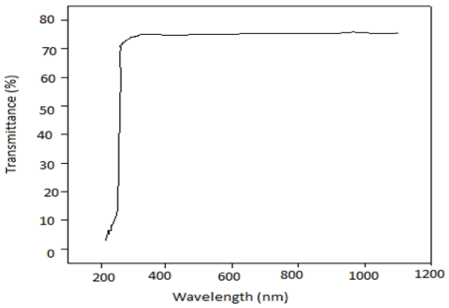

Figure 4: Transmittance spectrum of gamma-glycine crystal doped with 1 mole% of L-arginine

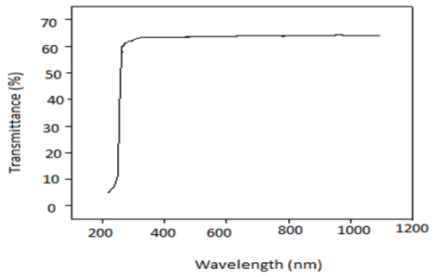

Figure 5: Transmittance spectrum of gamma-glycine crystal doped with 3 mole%of L-arginine

Table 3: Values of band gap energy for undoped and doped gamma-glycine samples

Sample	Band gap (eV)
Undoped gamma-glycine	5.62
Gamma-glycine + 1 mole% of L-arginine	5.01
Gamma-glycine + 3 mole% of L-arginine	4.97

CONCLUSION

Various properties of gamma-glycine have been improved by adding dopant L-arginine. The solubility and induction period of L-arginine doped gamma glycine samples have been experimentally determined.XRD methods were used to determine the crystal structure of the grown crystals. From the results, it is concluded that pure and dopedgamma-glycine are observed to be crystallizing in hexagonal structure. The slight alteration in the values of lattice constants of doped NLO crystals is due to incorporation of dopants into the host crystals.In order to characterize the grown crystals spectroscopically, FTIR, UV-visible spectral studies have been carried out. The functional groups of the grown crystals have been identified and the absorption frequencies were changed slightly in the case of undoped and doped gamma-glycine crystals.

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