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Glycine Lithium Nitrate Doped with Sodium and Potassium Nitrates: Synthesis and Characterization

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ABSTRACT

Growing crystals can be done most simply via slow evaporation. When a guest molecule occludes the pure crystals of centrosymmetric glycine, Second Harmonic Generation (SHG) occurs. Amino acid-derived non-linear optical (NLO) materials areadvantageous in second harmonic generation. A solitary glycine crystal in the presence of trace amounts of sodium, potassium, chloride, bromide, lithium, and potassium nitrate are suitable non-linear optical (NLO) materials. Glycine lithium nitrate crystals have been produced using the slow evaporation method. Slow evaporation is used to form crystals of glycine and lithium nitrate, which are then doped with varying amounts of sodium and potassium nitrates (20%, 30%, 50%, and 60%).Crystallinity and functional group of the grown crystal have been identified by FTIR investigations. Optical band gap has been determined by UV method. The production of distinct spectra has been discussed on the basis of absorbency by the grown crystals.

Keyword: Slow evaporation method, UV, FTIR

I. INTRODUCTION

Research in a number of fields, including diode laser, optical communication, harmonic creation, laser lithography, and frequency mixing, has been sparked by the discovery of extraordinarily effective NLO materials. Organic materials have garnered a lot of attention due to their broad transparent window, thermal stability, strong nonlinear response, ease of synthesis, rapid nonlinear response, and promise for a wide range of device manufacturing. Additionally, they have been created and incorporated into gadgets.A variety of non-linear optical (NLO) applications for glycine's semi-organic single crystals have been evidenced. These crystals have been widely used in several optoelectronic technologies, including light modulation, laser crystals, optical memory storage, and optical amplifiers. In a similar manner, single crystals are separated into three groups: semi-organic materials, inorganic materials, and organic materials.

Numerous isolated amino acids bind together to generate metal-organic complexes. Semi-organic crystals can be created by combining amino acid as a ligand with transition metal ions.Due to their polarity, certain metal compounds containing amino acids display ferroelectric characteristics.The prospective uses of the NLO material for second harmonic production in optical information processing, optoelectronics, photonics, frequency conservation, and optical commuting piqued the interest of the condensed matter community.The complex of organic and semi-organic NLO materials is produced by amino acids, which are non-organic linear materials with a second harmonic conversion efficiency of non-linear optics. A single crystal of glycine can include good nonlinear optical (NLO) materials in the presence of minuscule quantities of potassium, sodium, chloride, and bromide. For many device applications, crystals with clear infrared and ultraviolet characteristics, high conversion efficiencies for second harmonic generation (SHG), and nonlinear optical properties are crucial. The arrangement of defects during crystal formation has a major impact on a material's optical, electronic, and electrical capabilities.

II. SAMPLE PREPARATION AND CRYSTAL GROWTH

Lithium nitrate and glycine were administered as a powder along with deionised water for the crystal formation. The glycine lithium nitrate crystals were produced in an aqueous solution using a slow evaporation approach, in which evaporation is allowed while the saturated solution is maintained at ambient temperature. To create an aqueous solution, 10ml of double-distilled water was mixed with glycine and lithium nitrate at a 4.5:1.5 mol ratio.

What manfilter paper was used to filter the prepared solution in a glass jar with a perforated cover. The compound was allowed to crystallize and a provision was established for gradual evaporation in a dust-free atmosphere. Tiny, colourless seeds were found after the solvent had evaporated from the saturated solution for four to five days.The mother solution was supplemented with doped materials at 20%, 30%, 50%, and 60%, respectively, to examine the effects of different kinds of impurities on the material's physical properties. These substances were nitrates of potassium and sodium. After 20 days, tiny seeds floating solution crystallize into a variety of shapes and sizes.

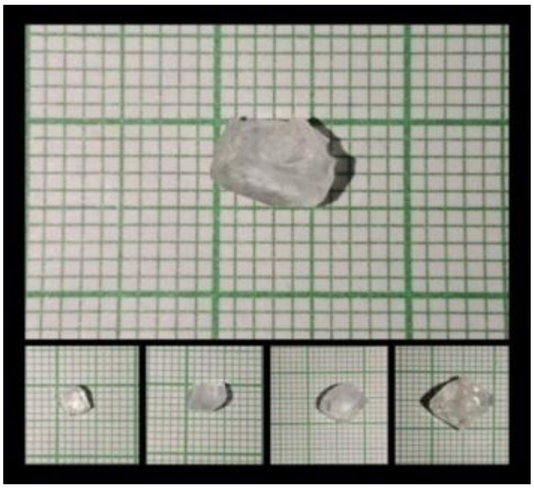


Figure.1 Glycine Lithium Nitrate doped with 20% , 30% , 50% and 60% of KNO_3

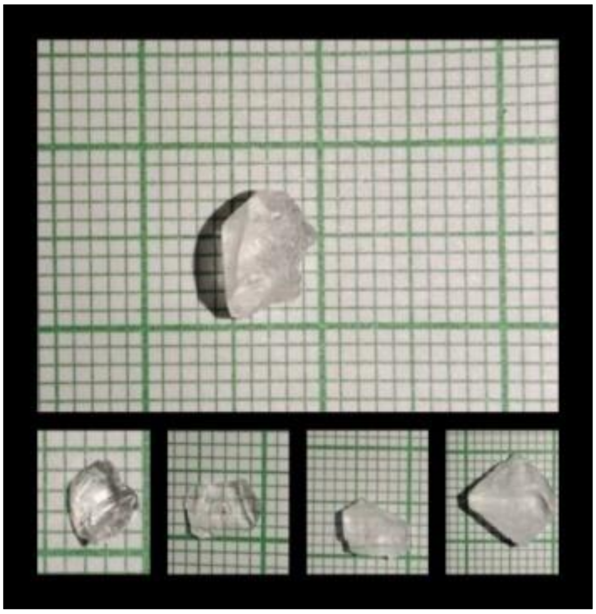


Figure.2 Glycine Lithium Nitrate doped with 20% , 30% , 50% and 60% $NaNO_3$

III.RESULT AND DISCUSSION

The mechanical, optical, and structural properties were investigated using pure crystalline crystals doped with KNO_3 and $NaNO_3$ at concentrations of 20, 30, 50, and 60%. Photon absorption or emission can be measured using UV-Vis absorption spectra. Using an FTIR spectrometer, an FTIR spectra was acquired in the wave number range of 450–4000 cm^{-1} to verify the existence of a functional group in the crystal lattice.

FTIR (FOURIER TRANSFROM INFRARED SPECTROSCOPY)

Transform of Fourier In order to confirm that there is a functional group in the crystal lattice, an infrared spectroscopy graph was recorded. Using an FTIR spectrometer, an FTIR spectrum in the 400–4000 cm–1 wave number range was obtained. The amount of infrared (IR) light that enters the material under study was noted. In actuality, each known chemical molecule has a typical infrared spectrum. The molecular structure of the structure under investigation can be inferred from the infrared spectrum. The O-H, C=O, and N-H symmetric stretching vibrations are correlated with the FTIR spectra.

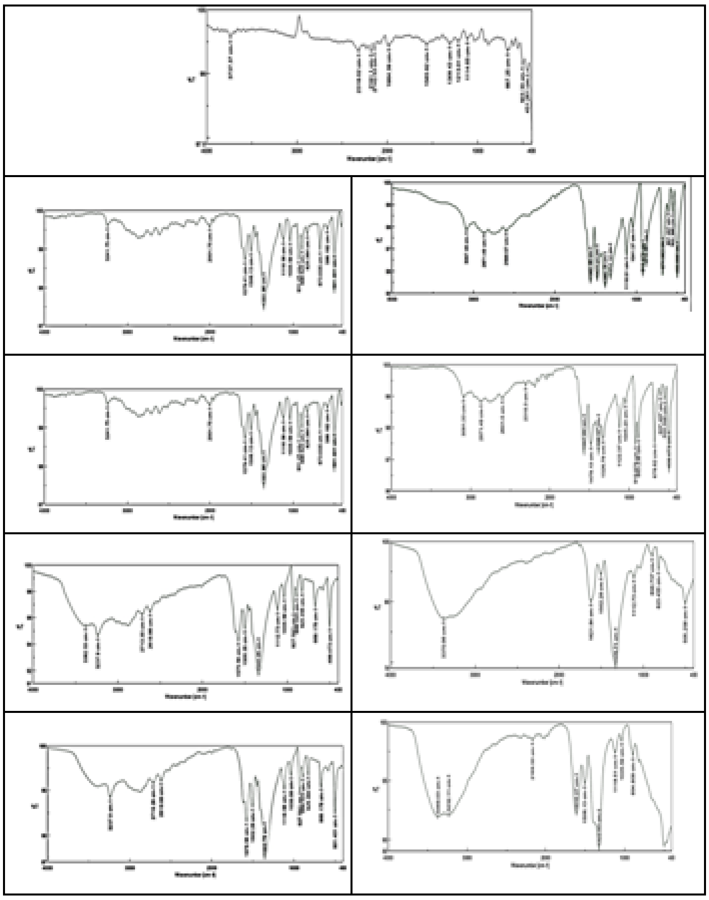


Fig. 5 FTIR of Glycine $LiNO_3$ doped with (A) undoped (B) 20% (C) 30% (D) 50% (E) 60% $NaNO_3$

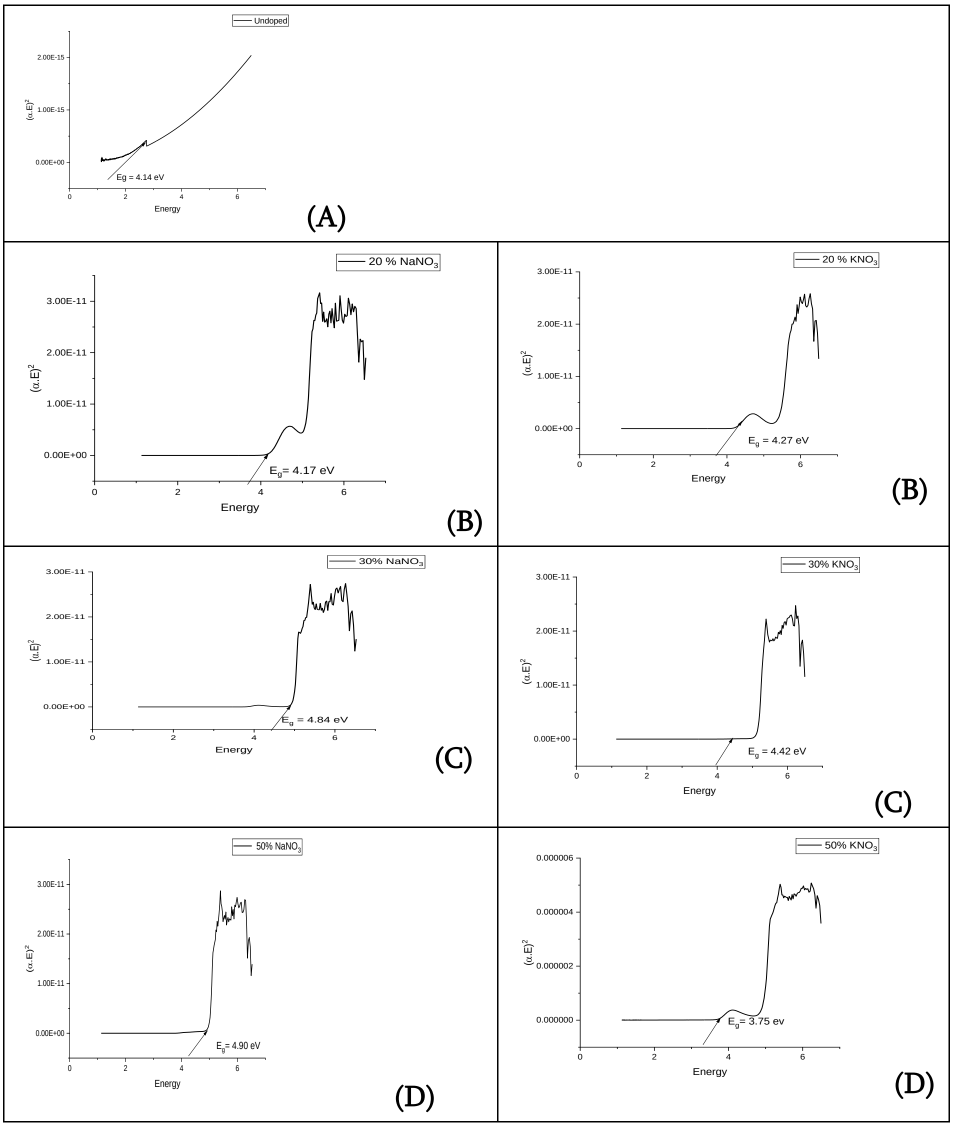
Fig. 6 FTIR of Glycine $LiNO_3$ doped with (A) undoped (B) 20% (C) 30% (D) 50% (E) 60% KNO_3

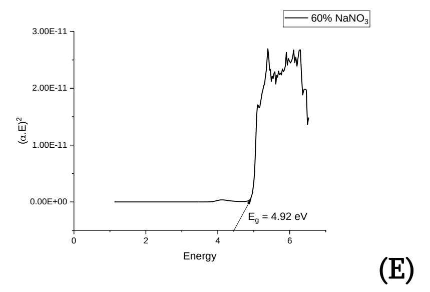
Undoped with $NaNO_3$			Undoped with KNO_3	
Sr. No.	**Wave number(cm^{-1})**	**AssignedVibration**	**Wave number (cm^{-1})**	**Assigned Vibration**
1	3382.53	N-H Group	3370.96	O-H Group
2	3241.75, 3237.9	=CH-H Group	2871.49	= CH_3 Group
3	2715.28, 2618.86	O-H Group	2601.5,2318.02	O-H Group
4	2142.53	C ≡ C Group	2181.1,2142.53	C≡C Group
5	1984.39	=C-H Group	1984.39, 1610.27	=C-H Group
6	1575.56, 1565.92	N-H Group	1565.92, 1502.28	C=C Group
7	1353.78,1340.28,	C-H Group	1328.71,1322.93	C-N Group
8	1213.01	O-H Group	1213.01,1122.37	C-O-C Group
9	1116.58, 1114.65,	C-O-C Group	919.87	O-H Group
10	931.45, 927.59	O-H Group	896.73, 894.80	=CH-H Group
11	673.03, 667.25	N-H Group	555.39, 505.25	C-Cl Group
12	503.33, 501.40	C - Cl Group	499.97, 451.26	C-I Group
13	499.47, 451.26	C- I Group	-	-

UV-Vis Absorbance Spectroscopy

The measurement of radiation absorption or emission linked to modifications in the spatial distribution of electrons in atoms and molecules is known as UV-Vis-NIR spectroscopy. In actuality, the electrons involved are typically the valence or bonding electrons, which are stimulated by UV, visible or near-IR light absorption. The spatial extent of the electron distribution is increased upon excitation of a bound electron from the highest occupied molecular orbital, resulting in a larger, more diffuse, and frequently more polarizable total electron density. A molecule that is vibrationally stimulated also has vibrational excitation. The intensity of spectral lines is determined by the likelihood of electronic transitions.

To have a large absorption cross section or a high likelihood of the molecule absorbing or emitting radiation, there needs to be a significant overlap between the vibrational modes in the initial and final electronic states. Within the initial and final electronic states, a broad variety of vibrational levels can result in electronic transitions. In the 200–1000 nm range, saturated hydrocarbons and molecules with just ether, alcohol, and alkyl groups exhibit transparency, or no absorption. These substances can be used as solvents for spectral determination when the specimen's solutions are used in this area.The UV–vis absorbance spectra of Glycine $LiNO_3$ doped with $KNO_3$and $NaNO_3$are recorded in order to determine the optical transparency of the formed crystal. The energy gap between the undoped and doped samples was computed using UV measurement data, and the results are shown in figures 3 and 4.





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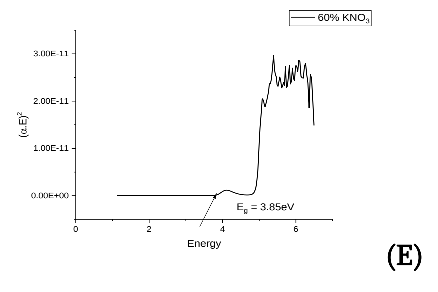

(E)

Fig. 3 Direct band gap of Glycine $LiNO_3$ doped with (A) undoped (B) 20% (C) 30% (D) 50% and (E) 60% $NaNO_3$

Fig. 4 Direct band gap of Glycine $LiNO_3$ doped with (A) undoped (B) 20% (C) 30% (D) 50% and (E) 60% KNO_3

Dopant= $NaNO_3$		**Dopant= KNO_3**	
Glycine $LiNO_3$	Band Gap (eV)	Glycine $LiNO_3$	Band Gap (eV)
Undoped	4.14 eV	Undoped	4.14eV
20%	4.17 eV	20%	4.27 eV
30%	4.84 eV	30%	4.42 eV
50%	4.90 eV	50%	3.75eV
60%	4.92 eV	60%	3.85 eV

IV. CONCLUSION

The usual slow evaporation method with double-distilled water at room temperature was used to successfully create the single crystal of Glycine $LiNO_3$ doped with KNO_3 and $NaNO_3$ with a 4.5:1.5 mol ratio. Regarding non-linear optical applications, it is a strong rival with enormous potential. FTIR spectroscopy research verified the molecule's molecular structure and the presence of the functional group. It is evident from a study of the direct energy band gap of crystals using UV Vis absorption spectroscopy that the band gap grows proportionately with the level of doping in the sample.

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