Investigation of Functional Group, Optical and Structural Characteristics of Doped and Pure Glycine $LiNO_3$ Crystals

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Abstract

Second Harmonic Generation (SHG) from the Centro-symmetric Glycine crystals in its pure form shows a photo-type of waves on resistance from the guest molecule. Second harmonic generation may benefit from the use of such Non-Linear Optical (NLO) materials. Slow evaporation is used to form a single crystal of glycine that is excellently optically transparent and has good nonlinear optical behaviour in a solution containing fractional amounts of sodium, potassium, and lithium nitrate. A diffractometer using Cu-Kα radiation was used to record the powder X-ray diffraction spectrum, which was scanned for eight minutes in the 85-degree range. When the lattice parameter values, particle size, dislocation density, strain values, and other factors are calculated. The paper studies exhibit the powder XRD pattern of the formed crystals. According to X-ray diffraction studies, grown crystals have very good crystalline perfection and no internal structural grain boundaries. In order to investigate structural phase, presence of different chemical bonds or additional elemental group etc. within grown crystals, they were examined by the spectrum of Fourier Transform Infrared (FTIR) spectroscopy. Assigned vibration of various chemical bond groups were identified and confirmed by this investigation. Optical Characteristics of Doped and Pure Glycine $LiNO_3$ crystals were carried out by visible and ultraviolet (UV) spectra and band gap (E_g) of the synthesized sample were calculated. For a nonlinear application, it was determined that the optical transparency and cut off wavelength needed to be equals to 300 nm. For $NaNO_3$ with concentration of 20% and 60% doping, the band gap was found as 6.07 eV and 5.84 eV respectively. For KNO_3 doping with concentration of 20% and 60%, the energy band gap was found to be 6.21 eV and 5.88 eV respectively.

Keywords: Grown from solution, Slow evaporation, Glycine $LiNO_3$, XRD, FTIR, UV-Vis spectroscopy.
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Introduction

Due to recent technological advancements, the optoelectronics industry has a strong need for optical single crystals and photonic fields. Such crystals are employed as devices for frequency conversion, high optical data storage etc. Glycine comes in three main types of polymers: α, β and γ. Centrosymmetric crystals of two polymorphic forms, α and β, with space groups are found as P_{21}/C and P_{21} respectively. On the other hand, γ glycine crystallizes in a non-centrosymmetric manner with a space group of P_{32}, which makes it a viable option for nonlinear applications. In the current study, a with the slow evaporation approach, a single crystal of glycine was created with the presence of $LiNO_3$ and its optical and mechanical properties were examined.

Method

At room temperature, a 4.5:1.5 ratio of glycine and $LiNO_3$ was made by dissolving it in deionized water. After stirring for around half an hour, the produced solution was filtered through filter paper. The saturation solution is maintained at room temperature in a dust-free environment in a petri dish that has been coated with perforated paper. Twenty days later, glycine lithium nitrate crystals are extracted. Following that, a solution of $NaNO_3$ and KNO_3 at concentrations of 20%, 30%, 50%, and 60% was prepared, and glycine $LiNO_3$ seeds were doped into it. Following 10 to 15 days, small and colourless crystals of Glycine $LiNO_3$ were extracted along with doped $NaNO_3$ and KNO_3 at 20%, 30%, 50%, and 60% of concentrations.

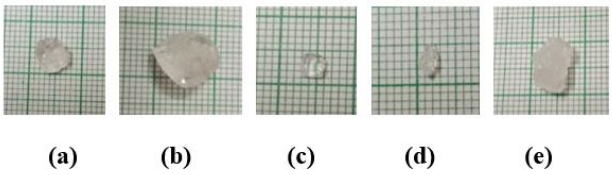


Figure 1: (a) Undoped Glycine $LiNO_3$, **(b)** to **(e)** doped with $NaNO_3$ of 20%, 30%, 50%, and 60%.

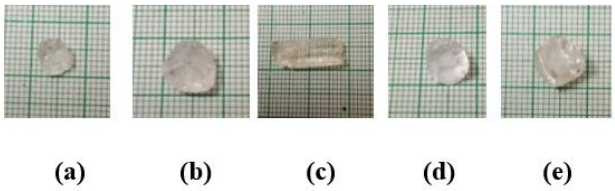


Figure 2: (a) Undoped Glycine $LiNO_3$, **(b)** to **(e)** doped with KNO_3 of 20%, 30%, 50%, and 60%.

Discussion

X-Ray Diffraction (XRD)

Using x-ray powder diffraction, the generated Glycine $LiNO_3$ pattern was obtained using a smart lab (3kw) powder x-ray diffractometer with CuKα (0.154 nm) radiation for structured analysis of the crystal. The ideal specimen was made by randomly orienting powder with crystallite size less than 10 μm concentrated with the probability distribution of crystalline orientation in polycrystalline materials. The diffraction angle (2θ), which is the angle between the incident and diffracted beams, can be altered to measure intensity and gather diffraction data by moving the tube, sample, and detector. Crushed crystal powder was scanned at a rate of 1° per minute within the 10-80° range.

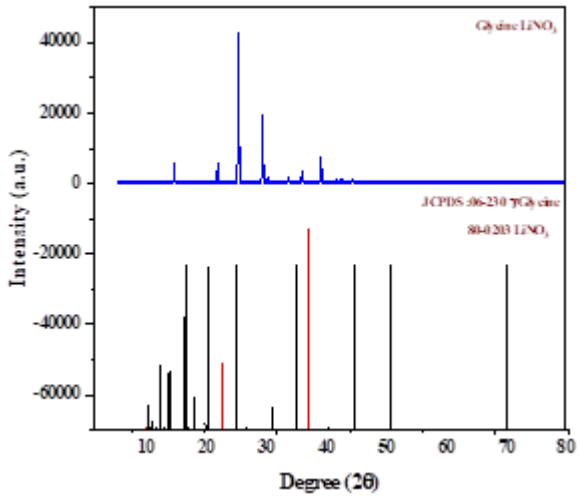


Figure 3: XRD graph of Glycine $LiNO_3$ with pure Gamma Glycine and $LiNO_3$

The JCPDS card number for Glycine and $LiNO_3$ indicates that the lattice parameter of the grown crystal is a = 7.024, b = 7.025, and c = 5.472 for Glycine. The value of α and β = 90°and γ = 120° indicates that the crystal structure is hexagonal. When the values of a, b, and c for $LiNO_3$ are 4.692, 5.034, and 15.21, and the values of α and β = 90° and 120°, respectively, the crystal structure is hexagonal which is shown in table1.

Table 1: Unit cell parameter of Glycine $LiNO_3$ Crystal

Lattice parameter	Glycine	Lithium Nitrate
a ($\dot{A}$)	7.024	4.692
b ($\dot{A}$)	7.025	5.034
c ($\dot{A}$)	5.472	15.21
α	90°	90°
β	90°	90°
γ	120°	120°
Crystal System	Hexagonal	Hexagonal
Space group	P_{31} (144)	R $\bar{3}$c (167)
Volume	233.80	290.08

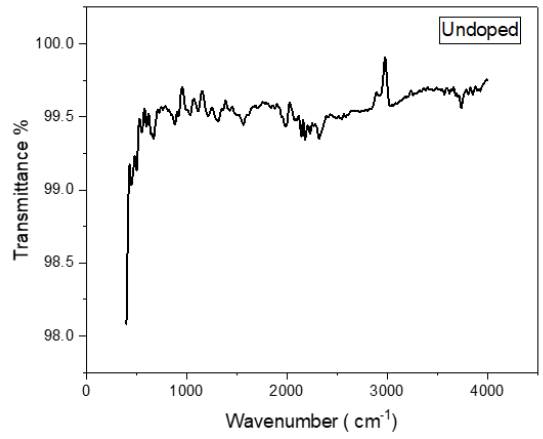
Table 2: Powder XRD Data of Glycine $LiNO_3$ Crystal

2θ°		d-Spacing (Å)		hkl	References
Observed Value	Standard Value	Observed Value	Standard Value		
14.58	14.54	6.0698	6.0800	100	JCPDS Card No. 06-0230 80-0203
21.83	21.81	4.0644	4.0700	101	
25.32	25.34	3.5142	3.5100	110	
29.34	29.35	3.0078	3.0400	200	
30.18	30.25	2.9574	2.9500	111	
33.65	33.65	2.6217	2.6600	201	
35.93	35.88	2.4554	2.5000	102	
39.12	39.12	2.2554	2.3000	210	
42.51	44.58	2.0370	2.0300	300	
44.46	44.58	1.9850	2.0300	300	

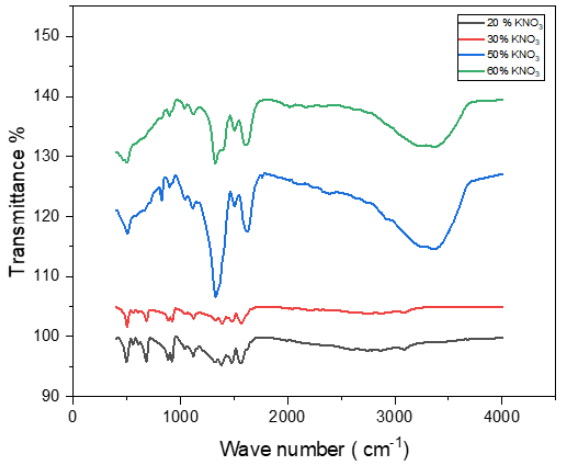
Fourier Transform Infrared Spectroscopy (FTIR)

Glycine $LiNO_3$ doped with $NaNO_3$ and KNO_3 in a range of concentration-wise tests can qualitatively identify the existence of functional groups in a molecule. The FTIR spectra were obtained between range of 4000 cm^{-1} and 400 cm^{-1}. The different absorption peaks were found in FTIR

spectra for both pure glycine $LiNO_3$ and 20% doped $NaNO_3$ and KNO_3.



(a)



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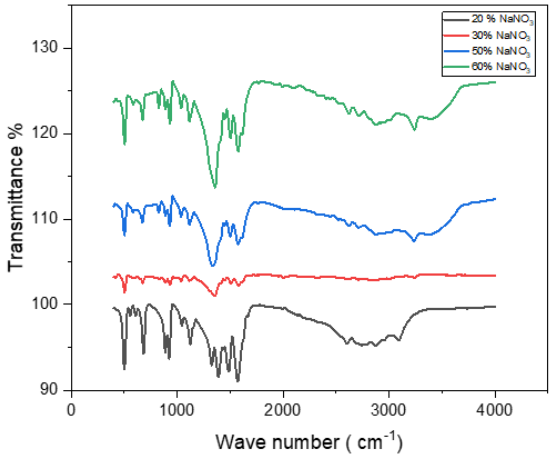


(c)

Figure 4: (a) Glycine $LiNO_3$, **(b)** doping with $NaNO_3$ and **(c)** doping with KNO_3

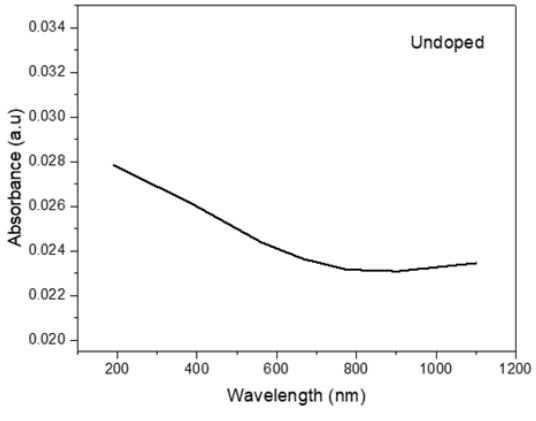
This work provides information on the molecular structure of the created molecule, which aids in the explanation of chemical bonding. There is a specific infrared spectrum for each chemical substance. IR detected in the range of 1340.28 cm^{-1} to 1353.78 cm^{-1}, which is consistent with the existence of the C-H group. There are observed degenerate modes of stretching vibration for N-H, C≡C, C=O, O-H.

Table 3: Wave numbers with assigned vibration of FTIR

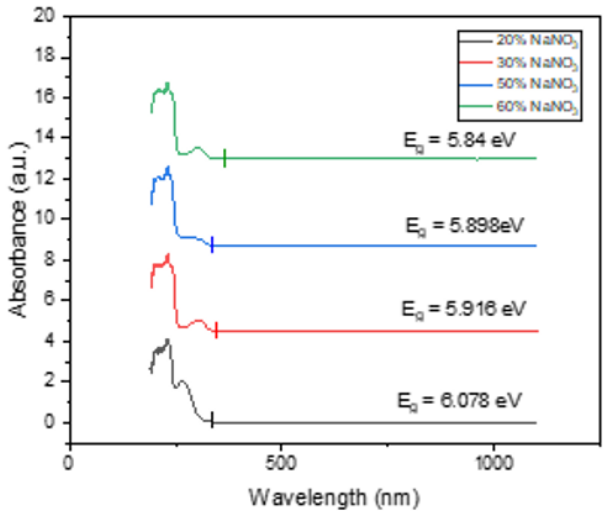
Sr. No.	Wave number (cm^{-1})	Personalized Vibration	Wave number (cm^{-1})	Personalized Vibration
1	3382.53	N-H Group	3370.96	O-H Group
2	3241.75,3237.9	=CH-H Group	2871.49	$=CH_3$ Group
3	2715.28,2618.8	O-H Group	2601.5, 2318.02	O-H Group
4	2142.53	C≡ C Group	2181.1, 2142.53	C≡ C Group
5	1984.39	=C-H Group	1984.3, 1610.27	=C-H Group
6	1575.56,1565.9	N-H Group	1565.9, 1502.28	C=C Group
7	1353.78,1340.2	C-H Group	1328.7, 1322.93	C-N Group

UV-Vis Spectroscopy

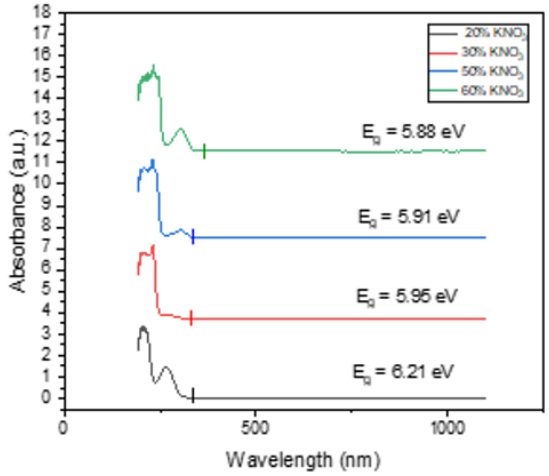
For optical transmission of Glycine $LiNO_3$ crystal with doped sample are measured in range of 200-1100 nm using UV-Vis spectrometer. A band gap is not observable when measured in the pure Glycine $LiNO_3$ graph with a UV-vis analysis. A study of a comparable graph of Figure 5 (a) and (b) shows that band gaps arise whenever pure material is subjected to a doping concentration. At 20% and 60% doping concentrations of $NaNO_3$, the energy band gap is 6.07 eV and 5.84 eV respectively. For KNO_3, the energy band gap at 20% is 6.21 eV and at 60% of the doping concentration is 5.88 eV.



(a)



(b)



(c)

Figure 5: (a) UV-Vis spectroscopy graph of Glycine $LiNO_3$, **(b)** doped with $NaNO_3$, **(c)** doped with KNO_3

Table 4: Doping concentration of Glycine $LiNO_3$ doped with $NaNO_3$ and KNO_3

Concentration	$NaNO_3$	KNO_3
	Energy Band gap (eV)	Energy Band gap (eV)
Undoped	-	-
20%	6.07	6.21
30%	5.91	5.95
50%	5.88	5.91
60%	5.84	5.88

Conclusion and Future Prospective

Glycine $LiNO_3$ crystal structure was grown at ambient temperature via slow evaporation. Research employing UV-vis absorption spectroscopy has shown that a pure sample cannot have a band gap; however, when an impurity is added, the material starts to show a band gap, and the doping material's band gap shrinks as the concentration rises. XRD analysis confirmed that the structured type of crystal is HCP (Hexagonal Cubic Pack) and FTIR analysis confirmed the material's functional groups.

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