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Growth and characterization of glycine sodium nitrate crystals

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ABSTRACT

Good quality single crystals of glycine sodium nitrate a new semiorganic nonlinear optical (NLO) crystal has been successfully grown from aqueous solution by slow evaporation method. The structural characterization of the grown crystals was carried out by X-ray diffraction. The grown crystals were subjected to FTIR for vibrational assignments. The optical properties were studied for the SHG efficiency. It is found that the cutoff wavelength lies in the UV region. The mechanical response of the crystal has been studied using Vickers microhardness technique.

Introduction

Nonlinear optical (NLO) materials[1-5] have a significant impact on laser technology, optical communication and optical storage technology. The search for new frequency conversion materials over the past decade has led to the discovery of many semiorganic materials. Glycine and its isomorphs crystals have been subjected to numerous studies in the past 30 years, especially because of its excellent ferroelectric and pyroelectric properties. Amino acids are one of the best materials for use as a sensitive element in pyroelectric infrared sensors due to its high pyroelectric coefficient (p), reasonably low dielectric constant (ε) and best figure-of merit (p/ε). Pyroelectric sensors based on glycine are uniformly sensitive to radiations over wide wavelength range from ultra-violet to far-infrared, and operate at room temperature compared to quantum detectors, which require cooling.

Many efforts have been made in the past to understand the growth mechanism [6-15] and improve its pyroelectric, mechanical, optical, and ferroelectric properties and to prevent depolarization. Efforts are mainly focused towards understanding the growth mechanism, growth rate and modifying the desired pyroelectric properties by doping glycine crystals with inorganic and organic dopants[16-21]. The present work deals with material synthesis, investigations on growth of glycine sodium nitrate single crystals using water as solvent.

Synthesis of glycine sodium nitrate

The starting materials glycine and sodium nitrate (analytical grade reagents) were taken in the ratio 1:1. The calculated amount of salts was dissolved in deionized water at room temperature.

The calculated amount of glycine was first dissolved in the deionized water. Then sodium nitrate was added slowly to the solution with continuous stirring. The prepared solution was let to dry at room temperature. The purity of the synthesized salt was improved by the successive recrystallization process. Care was taken during heating of the solution and a maximum temperature of 40˚C was maintained in order to avoid decomposition. Fig. 1 shows the as grown crystal of glycine sodium nitrate with an optimized solution pH value of 3.8.

Powder X-Ray Diffraction Analysis

Finely crushed powders of glycine sodium nitrate were subjected to powder x-ray diffraction analysis were carried out using SEIFERT diffractometer with $CuK\alpha_1$ (λ = 1.5406 Å) radiation to identify the lattice parameters. The sample was scanned over the range 10-70 degree at a scan rate of 1 degree / min. The unit cell parameters evaluated from the diffraction data were a = 14.329 Å, b = 5.2662Å, c = 9.1129 Å and V = 600.9 $(Å)^3$ making an angle β of 119.10°. The crystallographic data is given in Table.1. The diffraction pattern is shown in Fig. 2. Fig. 3 represents the molecular packing of the glycine sodium nitrate in the unit cell.

FTIR Measurements

The Fourier transform infrared spectrum of the title crystal was recorded in the region 400 – 4000 cm^{-1} using Perkin Elmer Spectrum RX1 spectrophotometer equipped with He–Ne laser source, KBr beam splitter and $LiTaO_3$ detector. The sample was prepared by pressing GSN with KBr into pellet form. The observed spectrum is shown in Fig.4. The Vibrational assignment of glycine sodium nitrate were tabulated in Table 2. Thus, the molecular structure of the synthesized compound was confirmed by the spectral analysis.

Optical Properties of glycine sodium nitrate

The optical transmittance plays an important role in identifying the potential of the NLO material. Because the material can be of utility if it has wide transparency window With reduced absorption around the fundamental and second harmonic wavelength. The UV–vis transmittance has been performed using PerkinElmer Lambda 35 UV visible spectrophotometer in the region 200–1100 nm. The lower cutoff wavelength lies around 220 nm which is due to the π–π* transition in this compound. The reduction in absorption around Nd:YAG laser fundamental wavelength contributes the resistance of the material to laser damage threshold. The step decrease in transmittance around 220 nm may be assigned to electronic excitation in COO^- group. As there is no

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change in transmittance in the entire visible range up to 200 nm the materials can find application as window in spectral instruments in that region. Fig. 5 shows the optical transmission spectra of Glycine sodium nitrate

Fig 1. Grown crystal of glycine sodium nitrate

Table 1. Crystallographic data of glycine sodium nitrate

Identification code	**GSN**
Empirical formula	$C_2H_5N_2NaO_5$
Formula weight	160.07
Crystal structure	Monoclinic
Space group	Cc
Cell parameters	
a (Å)	14.329
b (Å)	5.2662
c (Å)	9.1129
α (˚)	90
β (˚)	119.10
γ (˚)	90
Volume (Å)^3	600.9
Z	4
Crystal size	20 x 14 x 7 mm^3

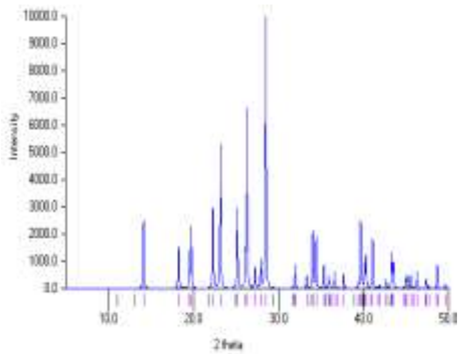

Fig 2. The diffraction pattern of the glycine sodium nitrate

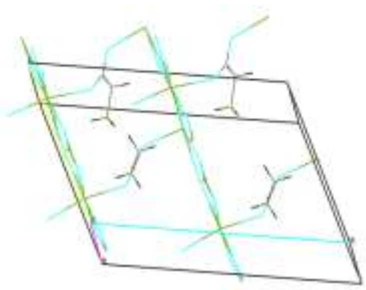

Fig 3. Molecular packing of the glycine sodium nitrate in the unit cell

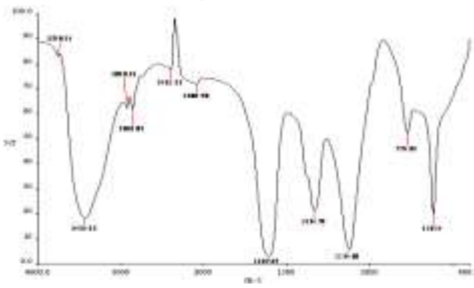

Fig 4. FTIR spectrum of glycine sodium nitrate

Table 2. Vibrational assignment of glycine sodium nitrate

FT-IR cm^{-1}	**Assignment**
3435	ν(NH)
2929 s	ν_s (NH_3^+), ν_s (CH_2)
1607 w	ν_{as}(COO^-), δ_{as}(NH_3^+)
	ν_{as}(COO^-)
1334 ms	ν_s(N=O)
1124 w	ν(C-O)
1090 w	ν_{as}(C-C-N), β (C-H)
1030 w	ν_{as}(C-C-N)
993 vs	ν(C-N)
774 vw	ν_s(COO^-),ν_s(C-C-N)
	ν(O-N-O)
619 w	ω(COO^-), ν(O-Na)

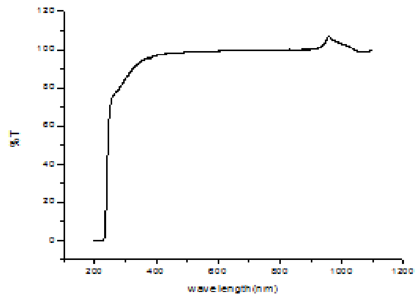

Fig 5. Optical transmission spectra of Glycine sodium nitrate

Vicker's Microhardness Studies

The Vicker's microhardness study uses a diamond pyramid indenter with an inclined angle of 136°. The Vicker's microhardness number against load (kg) was determined by actual area of impression (μm^2).

The value is independent of depth of penetration, as may be expected, since all indentations are geometrically similar. Vicker's microhardness number was then evaluated from the relation

$$H_v = \frac{1.8544\ P}{d^2} kg.mm^{-2}$$

where H_v is the Vicker's microhardness number, P is the applied load and d is the average diagonal length of the indentation impression. Hv increases with increasing load. Test load above 200g develop multiple cracks on the crystal surface due to the release of internal stress generated locally by indentation. Mechanical behaviour of Glycine sodium nitrate is shown in the figure .6.

Conclusion

Glycine sodium nitrate was synthesized by the reaction of glycine and sodium nitrate in water.

A single crystal was grown from the aqueous solution by slow evaporation method. FTIR confirmed the various molecular group vibrations and protonation of amino acids in the grown crystals. As there is no change in transmittance in the entire visible range upto 220nm, these materials can find application as window in spectral instruments in that region.

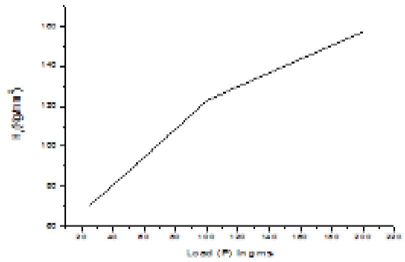

Fig 6 Mechanical behaviour of Glycine sodium nitrate

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