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Growth and Simulation Study of Glycine Sodium Nitrate Non-Linear Single Crystal

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Abstract

The present study is designed to simulate and study the production of single crystals of semi-organic non-linear optical Glycine Sodium Nitrate (GSN) by using hyper6 software and experimentally by slow evaporation technique. This work has investigated the molecular properties of the crystals using the density functional theory to obtain the infrared spectrum of the crystal by simulation. The FTIR investigation of growing crystal has shown that the spectrum of the GSN crystal compared to simulation evaluation is similar; the only difference is in the range of 1.9% to 2.75% of wavelength peak values. The ultraviolet experimental measurement of the GSN molecule reveals the possibility of non-linear properties due to the spectrum cutoff in the wavelength peak of 301 nm. There was a significantly positive correlation between simulation and experimental assessment.

Keywords

Glycine Sodium Nitrate, Simulation, Crystal Growth, FTIR Spectrometer, UV-Spectrophotometer

1. Introduction

Recently, attention has been focused on a variety of approaches of non-linear optical material interaction of electromagnetic radiation needed for spectroscopy of visible light, infrared, and ultraviolet radiation spectra [1]. The glycine sodium nitrate (GSN) crystal of second harmonic generation phenomena and laser photons formed by the interaction with non-linear material effectively joint to produce twice the photon energy, frequency, and half the wavelength [2].

Therefore, sodium glycine nitrate is a semi-organic compound that has a crystalline feature of the mechanical, electrical, and optical properties transformed with doped materials [3]. Essentially the second harmonic generation behavior of GSN crystal is produced by the high energy of the laser and non-linearity of an optical property of material due to the characteristics of the wavelength and refractive index of the material under search. Thus, the physical and chemical characteristics with the number of electrons in the orbits of sodium nitrate ($NaNO_3$) and glycine ($C_2H_2NO_2$) are forming two refractive indices of the semi-organic compound, which enhances the nonlinear optical properties of the crystal. The GSN crystal fundamental interaction with higher intensity and energy of laser radiation is enhancing the nonlinear properties of crystal that mostly is a laser pulse power. The nonlinear crystal property in principle is conducted with the effect of induced polarization and light pass through the optical material [2]. The Maxwell equations in differential form can be used to define the nonlinear behavior of the crystal.

$$\nabla \times E = -\frac{\partial B}{\partial t} \tag{1}$$

$$\nabla \cdot E = \frac{\rho}{\varepsilon_0} \tag{2}$$

$$\nabla \cdot D = \rho \tag{3}$$

$$\vec{D} = \varepsilon_0 \vec{E} \tag{4}$$

$$\nabla \times H = J + \frac{\partial d}{\partial t} = J + \frac{\partial \left(E + P_L + P_{NL} \right)}{\partial t} \quad \text{Ampere Maxwell law} \tag{5}$$

where the magnetic field (H or B) and electric field (D or E), J; microscopic charge density and ρ is charge function. D is the electric displacement field, E; the electric field, P_L; the linear polarization and P_{NL}; nonlinear polarization. The nonlinear phenomena of the crystal molecule can be defined by the following total polarization relation [2].

$$P_{tot} = \mu + \varepsilon_0 \left(P_L E_1 + P_{NL} E_2 \right) \tag{6}$$

where P_{tot} is the total polarization of the molecule, μ: the permanent dipole moment and ε_0 : permittivity of vacuum.

The Glycine Sodium Nitrate (GSN) has been grown from three different pH (1.1, 6.0, and 10.8) solutions by evaporation solution growth, which indicates the nonlinear optical (NLO) property that varies with the change in the pH values S. Palaniswamy and O.N. Balasundaram (2009). S. Suresha *et al.* in 2010 studied the properties of producing single crystals of Glycine Sodium Nitrate (GSN) and the density measurements were carried out by both theoretical and experimental methods [4] [5]. The slow evaporation technique is used to grow (SHG) crystal by c-glycine from aqueous solutions of a glycine and potassium bromide that the single crystals of organic nonlinear optical material at room temperature, Sd. Zulifiqar Ali Ahamed a. *et al.* (2013). Nickel Ni^{+2} has been added to a single

crystal of glycine potassium sulfate (GPS), which grows by slow evaporation technique that measured by XRD and Fourier transform infrared (FTIR), and the nonlinear optical (NLO) property tested by Kurtz and Perry powder technique, A. Karolin *et al.*, 2013 [6].

Glycine oxalic acid (GOA) was grown by slow evaporation method in 2 to 3 weeks' time and the NLO study using Nd:YAG laser shows significant conversion efficiency for a sample with the change in concentration of oxalic acid and transparency between 188 nm to 700 nm, Dr. Jyotsna R Pandey (2014) [7]. Semi-organic nonlinear optical crystals have been grown by the slow evaporation method using potassium nitrate (KNO3) doped glycine sodium nitrate (GSN). The functional group of the samples examined using Fourier Transform Infrared (FTIR) and second harmonic generation (SHG) efficiency measures by Kurtz-Perry technique, D. Dooslin Mary, 2015 [8]. Single crystals of glycine sodium sulfate (GSS) grown by a free evaporation method and the Ni^{+2} addition to the group increase the optical transparency and decrease the second harmonic generation efficiency (A. Karolin *et al.*) [9] [10]. D. Dooslin Mary *et al.*, was used as a method of gradual evaporation to grow semi-organic glycine sodium nitrate (GSN) is doped with lithium nitrate to produce pure crystals of nonlinear optical property 2015. Semi-organic nonlinear optical glycine zinc sulfate is a single-crystal physical property, investigated by Kurtz powder technique for second-harmonic generation in 2015 by Natarajan Nithyaa, Raman Mahalakshmib, Suresh Sagadevanc [11].

The material of non-linear characterizations is produced by applying the high intensity of laser energy of pluses mode in the infrared region, in which optical properties of nonlinearity are created in organic and inorganic compounds of good optical transparency phenomena [12]. However, GSN crystal is forming a second harmonic generation (SHG) of the wavelength of electromagnetic radiation in the IR region relative to the nonlinearity optical property [1]. However, Maxwell's differential equations obey the determination of the variation of the input function of the fields.

The density functional surface theory has been the dominant method for the quantum mechanical simulation of semi-organic non-linear optical Glycine Sodium Nitrate. The principal theory of the Hyper 6 simulation program is based on the concept of potential energy and that distinction between classical and quantum energies, kinetic, and potential energies. The energies of electrons exist versus the energies of nuclei that based on the Born-Oppenheimer approximation suggests that the nuclei are stationary, which solves for the electron motion and is studied as radiation emission [13]. This program provides an approach to define the problem of a potential energy surface for Glycine Sodium Nitrate and infrared spectrum of molecules. Consequently, the density functional theory (DFT) offers the molecular properties of the GSN and provides computations of doped inorganic and organic material system simulation. Therefore, DFT predicts a great variety of molecular properties such as molecular structures, vibrational frequencies, and atomization energies [14]. The second harmonic genera-

tion crystal structure assessment is obtained by simulation data in the optical properties of the semi-organic material. The GNS crystal material molecule designs using computer simulation and nonlinear optical properties that determine the data obtained and the particle geometry. The Gauss View molecules compound analysis program provides an approach to the problem of defining a potential energy surface and vibration modes for the motion of glycine sodium nitrate and infrared spectrum of molecules.

2. Experimental Method

The aims of the current study are the simulation and experimental growth of single crystals of semi-organic non-linear optical Glycine Sodium Nitrate (GSN). The pattern of the GNS crystal basis of simulation of molecular structure doped with inorganic compounds by using Hyper6 software that results in an infrared spectrum obtains the nonlinear of the optical crystal.

2.1. Hyper 6 Simulation

The glycine and sodium nitrate compounds of both molecules of GSN designed by modeling of the combination the atoms use the chemical equation ($NaNO_3$ + C_2H_5OH) is an impossible chemical reaction due to the complete electron shell of the atoms in the compound. The atoms were designed utilizing the program to investigate the infrared radiation effect on atomic structure. The principal theory of the simulation program uses to build the atomic and molecular compound and the Gauss View program is used to analyze the data on the concept of the potential energy of atoms and the distinction between classical and quantum energies, kinetic and potential energies. However, the density functional theory (DFT) has been the dominant method for the computer model simulation of non-linear optical glycine sodium nitrate.

2.2. Experiment

The growth of a single crystal of sodium nitrate ($NaNO_3$) and glycine ($C_2H_2NO_2$) is the basis of the fundamental interactions of electromagnetic radiation with materials, which is mainly related to material characterizations to get semi-organic non-linear optical crystal [15]. Equimolar of glycine and sodium nitrate were dissolved into deionized water under magnetic stirring. The aqueous solution was evaporated under slow evaporation at room temperature. After several weeks, a homogenous colorless sample crystal was grown in the solution, and crystallization of the GNS in a year period. The FTIR spectrometer is used to assess the simulation outcome of GNS molecular properties and qualitatively determine the functional groups of semi-organic materials. The experimental measurement of the infrared radiation spectrum of crystal was investigated using an FTIR spectrometer. UV-VIS spectrometer was used to carry out the analyses of the glycine sodium nitrate in ultraviolet radiation in the range of 220 nm to 1100 nm response to investigate nonlinear optical properties.

3. Results and Discussion

The simulation method used to investigate the molecular structure of glycine sodium nitrate forms a crystal is a well-established approach in second harmonic generation crystals. So, the datum used to assess the optical properties of semi-organic and the second harmonic generation of the crystal. The hyper 6 software program is used to build the glycine compound ($C_2H_5NO_2$) shown in Figure 1, which is displaying the atoms in the blue (N), 2 red (C), 2 Gray (O) color and 5 atoms of (H). In addition, the glycine infrared spectrum is displayed in Figure 2. The diagram in Figure 3 shows the sodium nitrate salt atomic compound ($NaNO_3$) and the molecule construction is three atoms of the red color of (O) and one atom of (N) and sodium (Na). The spectrum of sodium nitrate is displayed at the peak energies of the molecules in the infrared region in Figure 4. For the two compounds understudy the chemical formula is expressed below:

$$C_2H_5NO_2 + NaNO_3 \rightarrow C_2H_5NO_2 \cdot NaNO_3 \quad (7)$$

Figure 5 shows both compounds that diffuse and penetrate in liquid form and constitute the GSN crystal. The infrared spectrum simulation of glycine, sodium

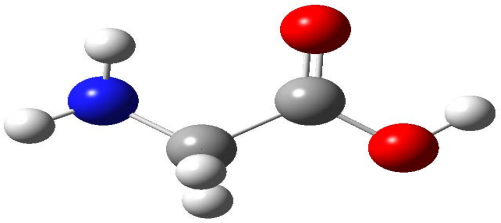

Figure 1. The diagram of glycine atoms the blue (N), 2 red (C), 2 Gray (O), and 5 atoms (H) and the optimization geometry of the compound.

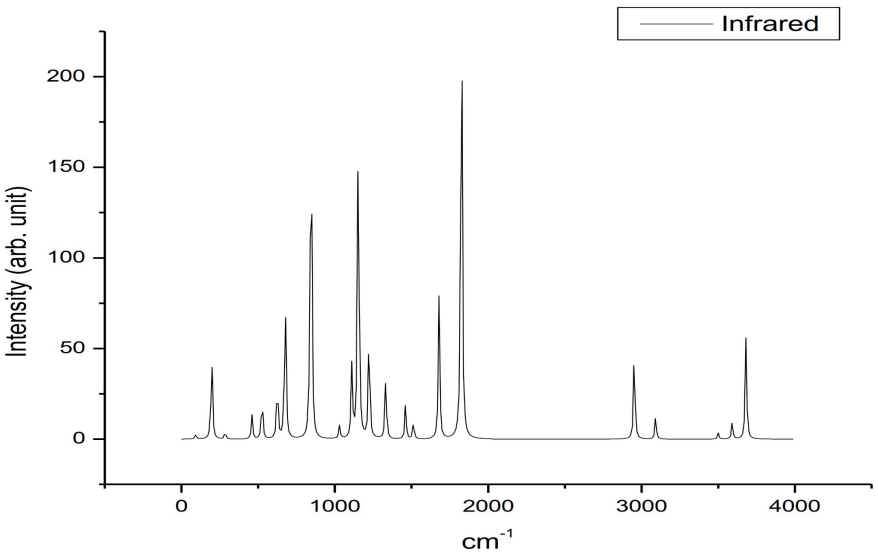

Figure 2. Infrared Fourier transform simulated spectrum of glycine. Sodium nitrate ($NaNO_3$).

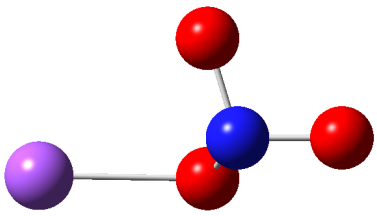

Figure 3. Shows sodium nitrate geometrical optimization diagram of the atoms combination appearance of 3 red (O), single blue (Na) and (N) atom.

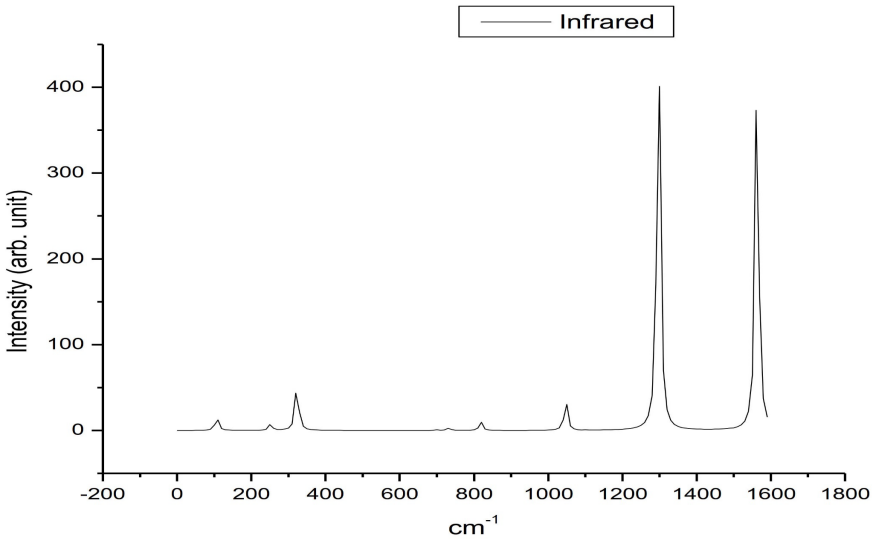

Figure 4. Shows sodium nitrate infrared Fourier transform spectrum.

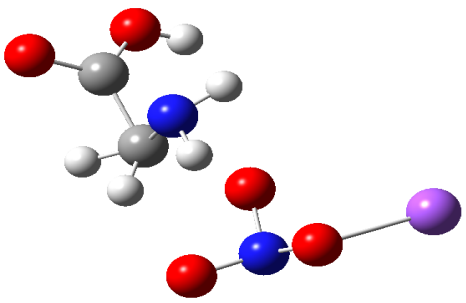

Figure 5. The structure of sodium glycine nitrate atoms is geometric optimization and displays the two compounds separately to construct the non-linear phenomena.

nitrate intensity peaks displayed in **Figure 6**. Picture of GNS sample of transparency appears in **Figure 7**. **Figure 8** displays the experimental measurement of GSN peaks of the IR spectrum is measured by FTIR spectrometer. **Figure 9** shows the ultraviolet spectrum of a sample using UVIS—spectrometer.

$$\text{Glycine } (C_2H_5NO_2) \tag{8}$$

$$C_2H_5NO_2{\cdot}NaNO_3 \tag{9}$$

As shown in **Figure 1**, the set of molecules glycine atoms, can be seen in the simulation FTIR intensities of the spectrum in **Figure 2**. The diagram in **Figure 3**

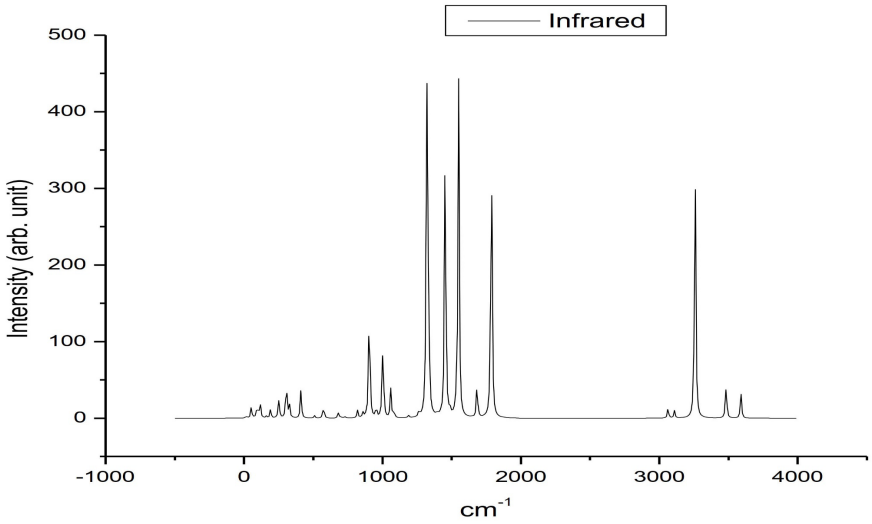

Figure 6. Glycine sodium nitrate infrared Fourier transform energy spectrum.

Figure 7. Show a picture of the glycine sodium nitrate crystal.

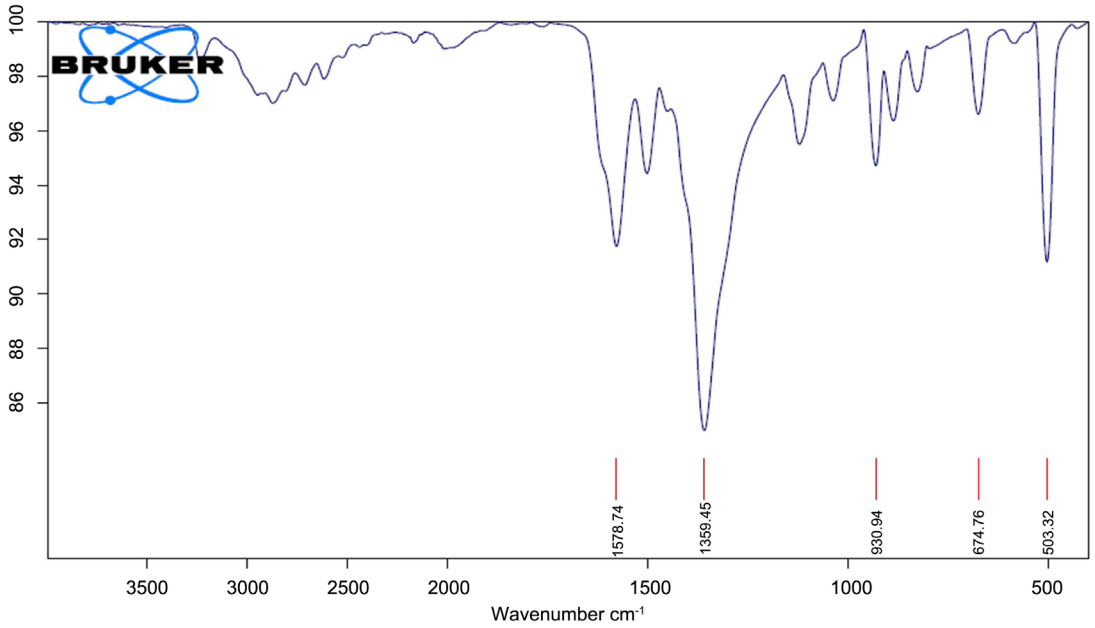

Figure 8. The experimental data of the spectrum on GSN measured by FTIR spectrometer.

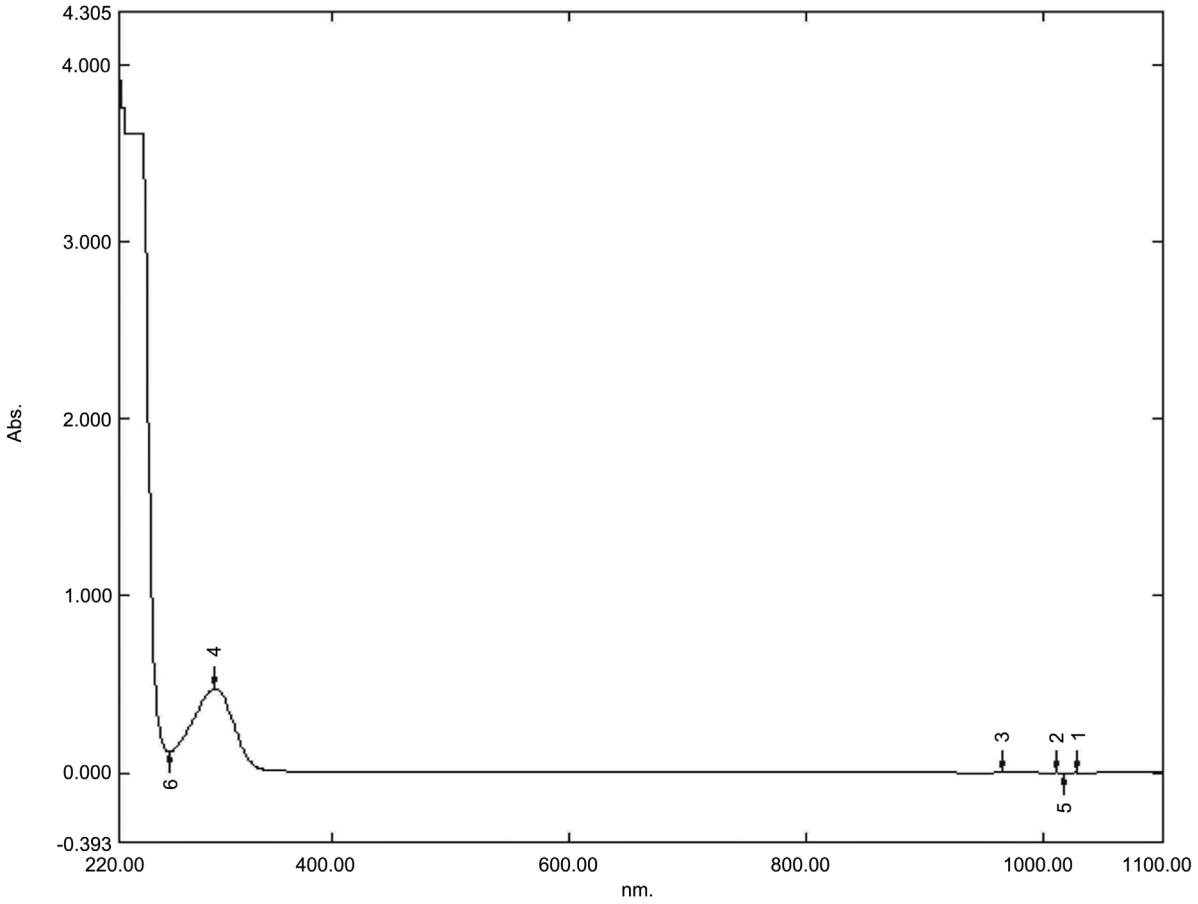

Figure 9. Spectrum of the ultraviolet spectrum of the sample using UVIS spectrometer.

shows the sodium nitrate salt atomic compound ($NaNO_3$) and the arrangement of molecules. The results obtained from the FTIR simulation of sodium nitrate a spectrum in **Figure 4**. The optical transparency of the crystal grown is becoming visible after the progress of the glycine sodium nitrate crystal formation in **Figure 7**. In order to assess the GSN crystal analyses, the infrared spectrum is compared to the simulation IR spectrum of the molecule to the relationship between two data. Interestingly, for GSN crystal wavelengths infrared spectrum was detected with the FTIR spectrometer measured the sharp wavelength peaks at 1578.74, 1359.45, and 930.34 cm^{-1} in **Figure 6**, which is similarly detected in glycine, sodium nitrate, and GSN single-crystal simulation in the range of 1548.89, 1322.6 and 904.006 cm^{-1} FTIR spectra.

In the sample of GSN crystal FTIR spectrometer measurement, the IR spectrum is shown the wavelength peaks 1578.74 and 1359.45 cm^{-1} as an example equal to a simulation spectrum of peaks in 1548.89 and 1334.81 cm^{-1} that indicated the variation of the total peaks 1.99% to 2.75% average. From this data, we can see that experimentation and simulation of GSN crystal resulted in the infrared radiation wavelength sharp peaks similarly in intensity values of spectra.

The ultraviolet radiation was applied to the sample to investigate the second harmonic generation possible response to the glycine sodium nitrate compound

Table 1. The peak values of the wavelengths of the UV spectrum.

Peak no.	Wavelength (nm)	Intensity (abs)
1	1027.00	0.000
2	1010.00	0.000
3	964.00	0.001
4	301.00	4760.
5	1016.00	−0.002
6	262.00	0.118

characterization [8]. The UV.VIS spectrometer is used for measuring UV absorption spectra in the ultraviolet of GSN so that the low absorption in the wavelength region supposes to be the crystal of non-linear characteristics. The result, as revealed in **Table 1** provides peak values point in the spectrum, which indicates the wavelength cutoff of the GSN in 301 nm. The picture shows the colorless crystal and in **Table 1** wavelength peak of UV region and lower absorption values in the visible region, which indicates a nonlinear property of the crystal [16].

The production of single crystals, semi-organic non-linear optical Glycine Sodium Nitrate (GSN) by Simulation using hyper6 software and experimentally by slow evaporation technique is obtained in the form of molecular structure and solid sample transparent crystal. The experimental ultraviolet measurement of the GSN molecule reveals the possibility of non-linear properties because of the spectrum cut in the wavelength. However, the non-linear properties and the second harmonic generation of the crystal are present because of the GSN property relative to the refractive index.

4. Conclusions

The present study was designed to determine the nonlinear properties of GSN crystal using simulation programs and experimental work. It shows a reliable mixture of the compounds of sodium nitrate and glycine is forming the solid sample crystal. The results of this investigation show that the crystal grows under using the slow rate evaporation technique at room temperature and the crystal formation is a transparent shape. The study of the molecular properties of crystals using the functional theory of density to obtain the infrared spectrums compared to the experimental IR measurement is carried out with great precision.

The simulation results of the crystal IR agreed with the experimental IR-spectroscopy where the wavelength sharp peak intensities closely matched with a difference in the range of 1.9% to 2.75%. GSN spectrum in the ultraviolet of the crystal of low cutoff wavelengths at the peak 301 nm and FTIR simulation and experimental measurement is likely non-linear for properties and second harmonic generation of the crystal.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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