



Spectral and Antimicrobial Activity Studies on Bis Glycine Hydro Bromide Semi-Organic Crystal

Muthuselvi C^{1*}, Sumathi B², Ravikumar B¹

¹Department of Physics, Devanga Arts College, Aruppukottai- 626 101, Tamilnadu, India

²Department of Physics, Madurai Kamaraj University Evening College, Madurai- 625002, Tamilnadu, India

Abstract The crystal of bis glycine hydro bromide was harvested from the slow evaporation method at room temperature and it was subjected to the single crystal XRD study for confirmation which ensures that the grown crystal has $P2_12_12_1$ space group with orthorhombic structure. The PXRD analysis shows crystalline nature of the title crystal. The various functional groups present in the crystal were analyzed by the FT-IR and FT-Raman spectroscopy techniques. The optical band gap was determined by the UV-Visible spectroscopy analyzes. The SEM with EDX analyzes shows that the grown crystal has smooth surface and well defined shape. The elemental composition study confirms the presence of elements in the title crystal. The antimicrobial activity of title crystal was tested against the four different micro-organisms by disc diffusion method. This result reveals that the parent and its complex crystals have no antibacterial effect.

Keyword: Bis glycine hydro bromide, XRD, antimicrobial activity, FT-IR, FT-Raman, SEM, EDX.

1. Introduction

Glycine is a white crystalline non-essential amino acid which was found in protein-rich foods such as meat, fish, dairy and legumes [1, 2]. Glycine is the derivative of acetic acid and it is also called as amino acetic acid [3]. Due to the addition of inorganic acids, it can easily crystallize. So it is termed as crystal friendly [4–5]. This simplest amino acid have three different polymorphisms (α -glycine, β -glycine and γ -glycine) [6-8]. In the past years, many researchers to grow glycine crystal with different combination of inorganic salts such as phosphoric acid [9], hydrofluoric acid [10], hydrobromic acid [11], nitric acid [12] and hydro chloric acid [13]. The structural studies of these amino acid complexes were reported by many authors [14,15]. Also, the crystal structure of bis-glycine hydro bromide was already reported by Natarajan et al. [16]. In the present work, single crystal XRD and powder XRD, FT-IR, FT-Raman, UV-Visible spectroscopy, SEM with EDAX studies were carried out. Apart from these, the antibacterial activity study seems to be enhanced because none of them were reported to this property for this compound.

2. Materials and Method

Materials

Commercially available raw materials of analar grade of glycine and hydro-bromic acid were purchased from the local scientific company, Madurai, India.



Methods

The bis-glycine hydro bromide single crystals were crystallized from the slow evaporation method. The equimolar ratio (1: 1) of glycine and hydro bromic acid were dissolved in deionized water. This solution was stirred for 1 hour and it was filtered using high quality filter paper. The filtered solution was poured into the petri dish. Now the petri dish was tightly closed with thick filter paper due to minimize rate of evaporation at room temperature. After a period of 15 days bulk transparent crystals were harvested and the photographic view of grown crystal is depicted in figure 1.



Figure 1: Grown crystal of bis glycine hydro bromide

3. Characterization Techniques

A good quality grown crystal of bis glycine hydro bromide were confirmed by single crystal X-ray diffraction analysis using Bruker SMART APEX CCD diffractometer with Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). The XPERT-PRO X-ray diffractometer with Cu K α ($\lambda = 1.54060 \text{ \AA}$) radiation was used to record the powder diffraction pattern. The FT-IR vibrational spectrum was recorded by using SHIMADZU FT-IR spectrometer in the range 4000-400 cm^{-1} . Also, the FT-Raman spectrum was recorded by using the BRUKER: RFS 27 Raman spectrometer in the wavenumber range 4000-400 cm^{-1} . The optical absorption spectrum has been recorded with SHIMADZU-UV1800 double beam spectrometer in the wavelength range 200-1100 nm in steps of 1 nm. The surface morphology and elemental analysis has been carried out by CARLZEISS EVO18 scanning electron microscope. The antimicrobial activity of parent and its complex crystals were tested against four different kinds of micro-organisms by disc diffusion method.

4. Results and Discussion

4.1. Single Crystal X-ray Diffraction

The unit cell dimension and space group of the title compound were determined from Bruker SMART APEX CCD single crystal X-ray diffractometer. For confirmation, these are checked with the Cambridge Structural Database (CSD) and the report showed that the grown crystal was exactly matched with already reported values [16]. The experimental values are tabulated in Table 1 and compared with the literatures [14, 15]. It is evident that the unit cell volume is high and close to the available literature [8]. The molecular structure of bis glycine hydro bromide crystal is shown in figure 2. In this crystal structure, the glycine molecule I exists in the zwitterion form $\text{NH}_3^+\text{CH}_2\text{COO}^-$ and the glycine molecule II exists in the cationic form $\text{NH}_3^+\text{CH}_2\text{COOH}$.

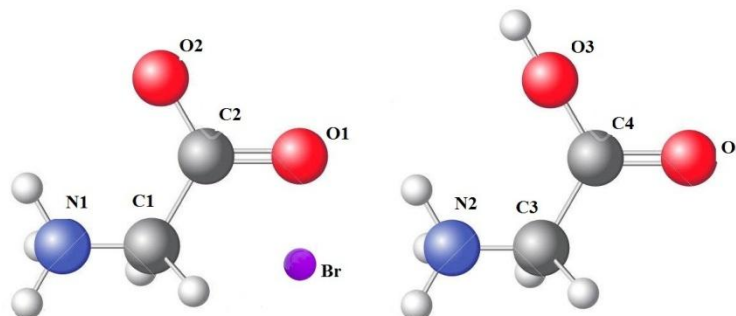


Figure 2: Molecular structure of bis glycine hydro bromide crystal



Table 1: Crystallographic data of bis glycine hydro bromide crystal

| Lattice Parameters | Present study | Already reported [16] |
|----------------------|--|---|
| Compound name | Bis glycine hydro bromide | Bis glycine hydro bromide |
| Empirical formula | C ₄ H ₁₁ N ₂ O ₄ ⁺ Br ⁻ | C ₄ H ₁₁ N ₂ O ₄ ⁺ Br ⁻ |
| Molecular weight | 231.05 | 231.05 |
| Unit cell Dimensions | a = 5.390(3) (Å) b = 8.198 (5) (Å) c = 18.416 (3) (Å) α = 90° β = 90° γ = 90° | a = 5.385 (1) (Å) b = 8.199 (2) (Å) c = 18.402 (3) (Å) α = 90° β = 90° γ = 90° |
| Volume | 816(Å) ³ | 812 (Å) ³ |
| Crystal system | Orthorhombic | Orthorhombic |
| Space group | P2 ₁ 2 ₁ 2 ₁ | P2 ₁ 2 ₁ 2 ₁ |

4.2. Powder XRD Analysis

The powder XRD pattern of the bis glycine hydro bromide crystal is shown in figure 3. The appearance of sharp and strong peaks confirmed the good crystallinity of the grown crystal. The characteristic peak of this compound has appeared at around 29.93°. The PXRD patterns are indexed using INDX software. The average crystalline size of title crystal was determined by using the Debye-Scherrer equation, which can be written as,

$$D = \frac{K\lambda}{\beta \cos\theta}$$

where,

D = average crystallite size

K = dimensionless shape factor (0.94)

λ = wavelength of X-ray radiation (Cu Kα = 1.54060 Å)

θ = diffraction angle

β = Full width at half maximum intensity

The Dislocation density can be calculated from,

$$\delta = \frac{1}{D^2} \text{ m}^2$$

where,

δ is dislocation density,

D is the crystallite size

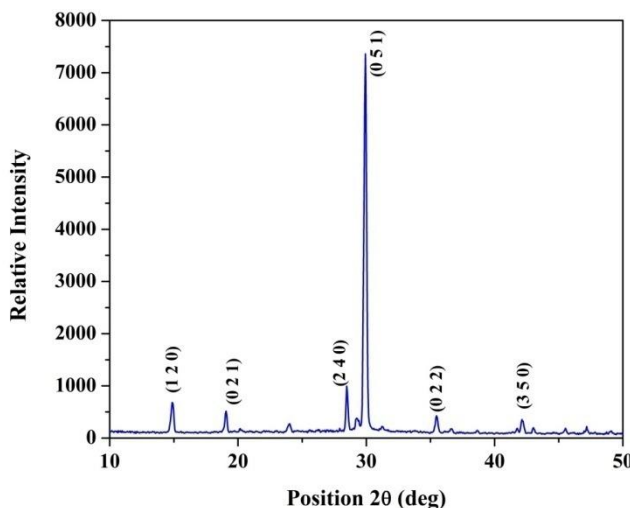


Figure 3: Diffraction patterns for bis glycine hydro bromide crystal



The average crystalline size is found to be as 33 nm for bis glycine hydro bromide crystal. Also, the dislocation density is determined as $8.96 \times 10^{14} \text{ m}^{-2}$.

4.3. Vibrational analysis

In bis glycine hydro bromide crystal structure, one glycine molecule has $[\text{NH}_3]^+$, COO^- and CH_2 functional groups and other glycine molecule has $[\text{NH}_3]^+$, COOH and CH_2 functional groups. The experimentally recorded FT-IR and FT-Raman spectra of title compound are shown in figure 4 and figure 5 respectively. The detailed wavenumber assignment for this compound is shown in Table 2.

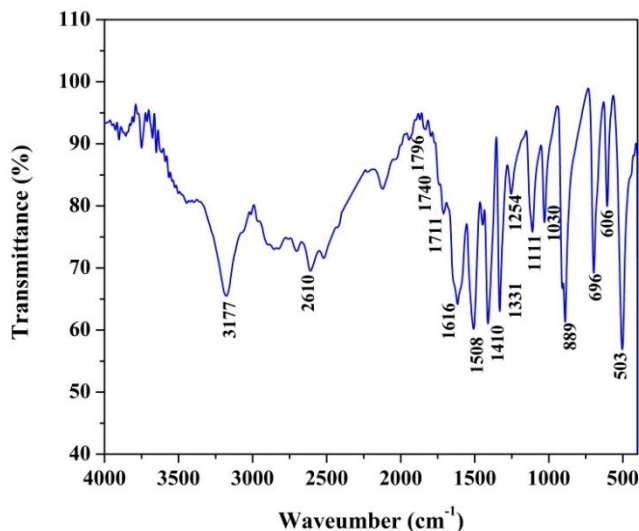


Figure 4: FT-IR spectrum of bis glycine hydro bromide crystal

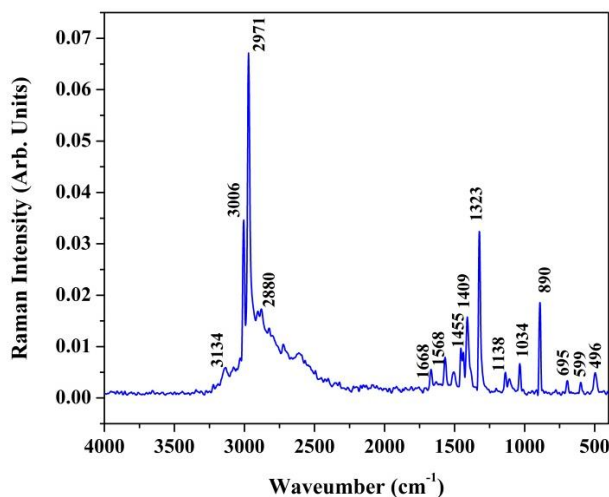


Figure 5: FT-Raman spectrum for bis glycine hydro bromide crystal

Table 2: Wavenumber assignments for bis glycine hydro bromide semi-organic crystal in FT – IR and FT – Raman spectra

| FT – IR ($\bar{\nu} / \text{cm}^{-1}$) | FT– Raman ($\bar{\nu} / \text{cm}^{-1}$) | Assignment |
|---|---|--|
| 3177 (s, br) | 3134 (m) | $\nu_{\text{as}}[\text{NH}_3]^+$ |
| 3010 (sh) | 3006 (m) | $\nu(\text{O-H})$ |
| 2980 (w) | 2971(s) | $\nu_{\text{s}}[\text{NH}_3]^+$; $\nu_{\text{as}}(\text{CH}_2)$ |
| 2884 (w) | 2880 (w) | $\nu_{\text{s}}[\text{NH}_3]^+$; $\nu_{\text{s}}(\text{CH}_2)$ |



| | | |
|-----------|----------|--|
| 1796 (w) | - | $\nu_{as}(C=O)$ |
| 1740(m) | - | $\nu_{as}(C=O)$ |
| 1711(w) | 1668 (w) | $\nu_s(C=O)$ |
| 1616(s) | - | $\delta_{as}[NH_3]^+$ |
| 1570(sh) | 1568(m) | $\delta_s[NH_3]^+$; $\nu_{as}(COO^-)$ |
| 1508(s) | 1506(w) | $\delta_s[NH_3]^+$ |
| 1447 (m) | 1455(m) | $\rho(CH_2)$; $\beta(O-H)$ |
| - | 1438(m) | $\beta(O-H)$ |
| 1410(s) | 1409(m) | $\beta(O-H)$ |
| 1331(s) | 1323(s) | $\nu_{as}(COO^-)$; $\omega(CH_2)$ |
| 1254(w) | - | $\nu(C-O)$; $t(CH_2)$ |
| 1140 (sh) | 1138 (w) | $\nu(C-N)$ |
| 1111 (m) | 1109 (w) | $\nu(C-N)$; $\nu(C-C)$ |
| 1030(m) | 1034 (w) | $\nu(C-N)$; $\nu(C-C)$ |
| 869(s) | 891(m) | $\gamma(O-H)$ |
| 696(m) | 696(m) | $\rho(COO^-)$ |
| 603(w) | 599 (w) | $\rho(COO^-)$ |
| 502(s) | 496(w) | $\rho(COO^-)$ |

$-[NH_3]^+$ group vibrations

The $-[NH_3]^+$ antisymmetric and symmetric stretching modes were found in the region of 3200 and 2800 cm^{-1} [17]. In the present study, antisymmetric stretching mode of $-[NH_3]^+$ group is identified as a strong broad band at 3177 cm^{-1} in IR and as a medium intensity band at 3134 cm^{-1} in Raman spectra respectively. Also $\nu_s-[NH_3]^+$ mode is attributed at 2980 cm^{-1} , 2884 cm^{-1} in IR 2971 cm^{-1} , 2880 cm^{-1} in Raman spectra. The deformation wavenumbers for the antisymmetric and symmetric mode of $-[NH_3]^+$ group were normally expected to fall in the region of 1625-1550 cm^{-1} and 1550-1505 cm^{-1} respectively [17, 18]. The $\delta_{as}-[NH_3]^+$ wavenumber is assigned at 1616 cm^{-1} in IR spectrum and the $\delta_s-[NH_3]^+$ band is attributed at 1570, 1508 cm^{-1} in IR and at 1568, 1506 cm^{-1} in Raman spectra in the present study. Due to the presence of hydrogen bonding network, the experimentally observed stretching and bending modes of $-[NH_3]^+$ group are deviated from the free ion.

COO⁻ group vibration

The characteristic ionized carboxylic group COO^- gives rise to antisymmetric and symmetric stretching modes in the regions 1600-1580 cm^{-1} and at 1400 -1280 cm^{-1} [19]. In the present work, the $\nu_{as}(COO^-)$ mode is attributed as a shoulder band at 1570 cm^{-1} in IR and as a weak Raman band at 1568 cm^{-1} . The symmetric stretching mode $\nu_s(COO^-)$ for this group is identified at 1331 cm^{-1} in IR and at 1323 cm^{-1} in Raman spectra respectively. The scissoring, wagging and rocking deformation modes of COO^- ionized carboxylic group were expected at 665 cm^{-1} , 577 cm^{-1} and 502 cm^{-1} respectively [19]. For the title compound these modes are assigned at 696 cm^{-1} , 603 cm^{-1} and 502 cm^{-1} in IR and at 695 cm^{-1} , 599 cm^{-1} and 496 cm^{-1} in Raman spectra respectively. These bands are assigned to the protonated carbonyl group of glycine molecule in cationic form.

CH₂ group vibrations

The CH_2 antisymmetric and symmetric stretching vibrations were exist in the region 3000–2900 cm^{-1} and 2900 and 2800 cm^{-1} respectively [20- 22]. Muthuselvi et al. [23] described the CH_2 symmetric stretching vibration for 6'-(3-Bromo phenyl)-7'-nitro-1',6',7',7a'-tetrahydro-3'H-spiro[indeno[1,2-b]quinoxaline-11,5'-pyrrolo[1,2-c]thiazole] molecule at 2929 cm^{-1} in IR and at 2942 cm^{-1} in Raman spectra for antisymmetric stretching mode of CH_2 group. Also, the symmetric stretching mode of the CH_2 group was assigned at 2871, 2867 cm^{-1} in both spectra. In the present work, bands are identified at 2980 cm^{-1} , 2884 cm^{-1} and at 2971 cm^{-1} , 2880 cm^{-1} in both spectra is assigned to $\nu_{as}(CH_2)$ and $\nu_s(CH_2)$ modes respectively. The CH_2 group bending modes wavenumber assignment orders are given



as follows: CH_2 scis > CH_2 wag > CH_2 twist > CH_2 rock [24]. The CH_2 scissoring, wagging and twisting modes fall in the range $1482\text{--}1437\text{ cm}^{-1}$, $1390\text{--}1180\text{ cm}^{-1}$ and $730\text{ cm}^{-1}\text{--}720\text{ cm}^{-1}$ respectively [23, 24]. In the present study, the absorption bands at 1447 cm^{-1} in IR and at 1455 cm^{-1} in Raman spectra is assigned to CH_2 scissoring mode. Also, CH_2 , wagging and twisting modes are attributed at the 1331 cm^{-1} , 1254 cm^{-1} (IR), 1323 cm^{-1} (Raman). The rocking mode is not identified for title compound. The vibrational wavenumbers for this group is not much changing which reveals that this group does not make any bonding with other groups.

C=O, C-O and O-H group vibrations

The antisymmetric and symmetric stretching wavenumbers of C=O group have IR band in the region $1720\text{--}1680\text{ cm}^{-1}$ and $1680\text{--}1640\text{ cm}^{-1}$ respectively [25]. In the present study, the bands occur at $1796, 1740\text{ cm}^{-1}$ in IR is assigned to $\nu_{\text{as}}(\text{C}=\text{O})$ mode. Also, bands at 1711 cm^{-1} in IR and 1668 cm^{-1} in Raman is assigned to the $\nu_{\text{s}}(\text{C}=\text{O})$ mode. The $\nu(\text{C}-\text{O})$ mode of carboxylic group normally occurs in the vibrational region of $1320\text{--}1210\text{ cm}^{-1}$ [26]. The title compound has the wavenumber at 1254 cm^{-1} in IR spectrum is attributed to $\nu(\text{C}-\text{O})$ mode. The O-H stretch from CO-OH group is identified at $3065\text{--}2826\text{ cm}^{-1}$ [23]. It is attributed at 3010 cm^{-1} in IR and at 3006 cm^{-1} in Raman spectra for title compound. The in- plane and out-of plane bending wavenumbers of O-H group appears in the region between $1440\text{--}1395\text{ cm}^{-1}$ and $960\text{--}875\text{ cm}^{-1}$ respectively [25, 26]. In the present work, $\beta(\text{O}-\text{H})$ mode is observed at 1447 cm^{-1} , 1410 cm^{-1} in IR and at 1455 cm^{-1} , 1438 cm^{-1} , 1409 cm^{-1} in Raman spectra respectively. Also $\gamma(\text{O}-\text{H})$ mode is attributed at 889 cm^{-1} , 891 cm^{-1} in both spectra of title compound. The presence of NH_3^+ , COO^- and COOH groups showed that bis glycine hydro bromide crystal has both cationic and zwitterionic nature.

Other vibrations

The C-C stretching and bending modes normally fall in the range $1117\text{--}870\text{ cm}^{-1}$ [27]. The C-N absorption bands for aliphatic amines appear in the region of $1250\text{--}1020\text{ cm}^{-1}$ [27]. In the present study the bands identified at 1111 cm^{-1} , 1030 cm^{-1} , 869 cm^{-1} in IR spectrum and at 1109 cm^{-1} , 1034 cm^{-1} in Raman spectrum is assigned to the $\nu(\text{C}-\text{C})$ mode of title compound. Also, the $\nu(\text{C}-\text{N})$ mode is attributed at 1140 cm^{-1} and 1138 cm^{-1} in both spectra. The other bands assigned to this mode mixed with C-C stretching vibration.

4.4. Optical analysis

The absorbance spectrum of title crystal was obtained by using SHIMADZU-UV1800 double beam spectrometer in the wavelength range $200\text{--}1100\text{ nm}$. The experimentally recorded absorbance spectrum is shown in Figure 6. The lower cut-off wavelength is found to be at 230 nm . The title crystal has 100% transmittance in the entire visible region which makes usefulness of this material in optical application.

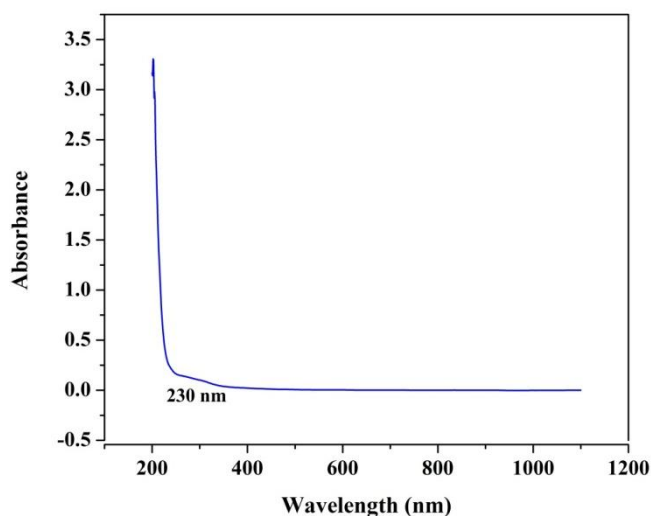


Figure 6: Absorbance spectrum for bis glycine hydro bromide crystal



The energy gap E_g is determined by using the Tauc's relation $(\alpha h\nu)^2 = A(h\nu - E_g)$ by plotting the $(\alpha h\nu)^2$ Vs photon energy and extrapolate the linear portion of $(\alpha h\nu)^2$ to the photon energy axis gives the energy gap value of bis glycine hydro bromide crystal.

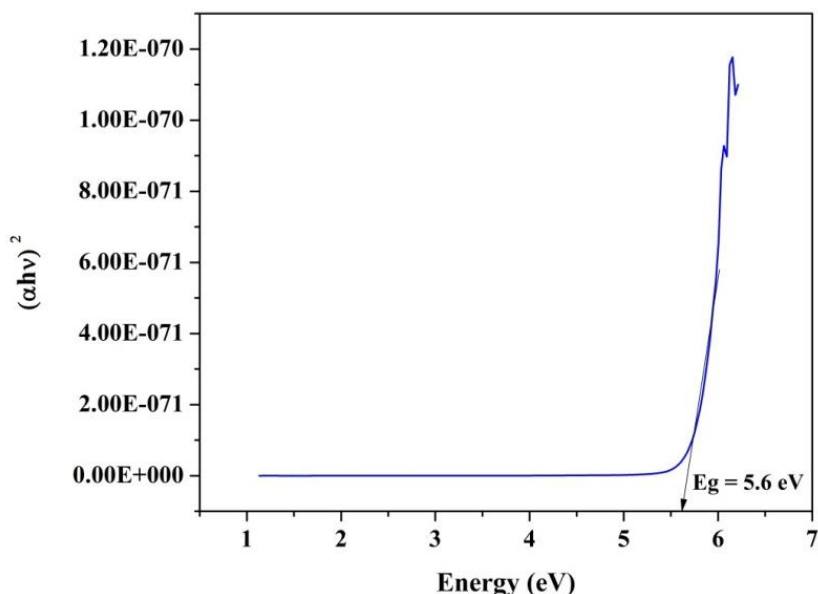


Figure 7: Optical band gap for bis glycine hydro bromide crystal

It is found at 5.6 eV from the Figure 7 and this study reveals that the grown crystal is a typical of dielectric material.

4.5. SEM with EDX Analyzes

The morphology and elemental analyzes of the title crystal were performed by SEM with EDX analyzes. The SEM images of title crystal with two different magnifications are illustrated in Figure.8. This image reveals that the grown crystal has small voids and porous nature in the surface which may be due to solvent inclusion. However, the major part of the crystal has well defined shape.

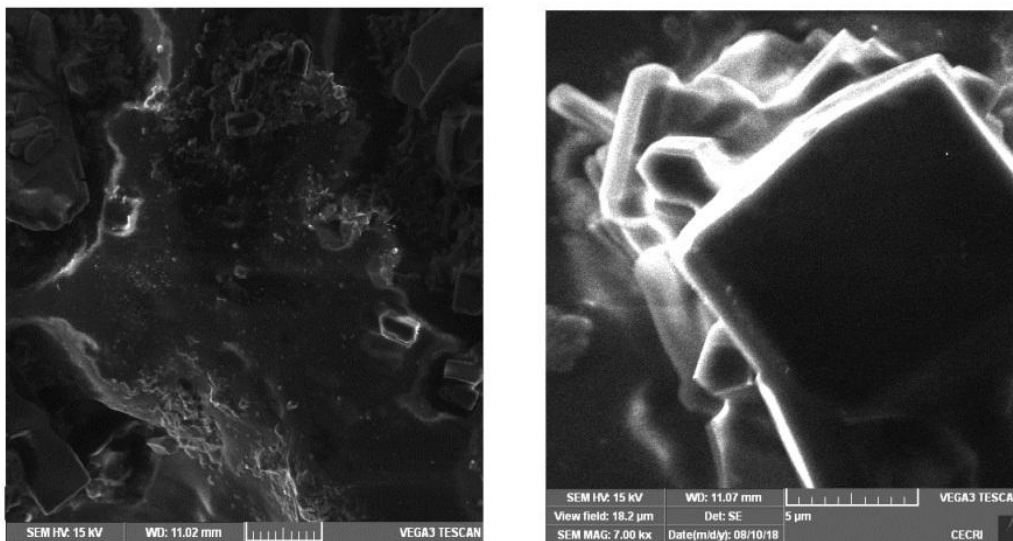


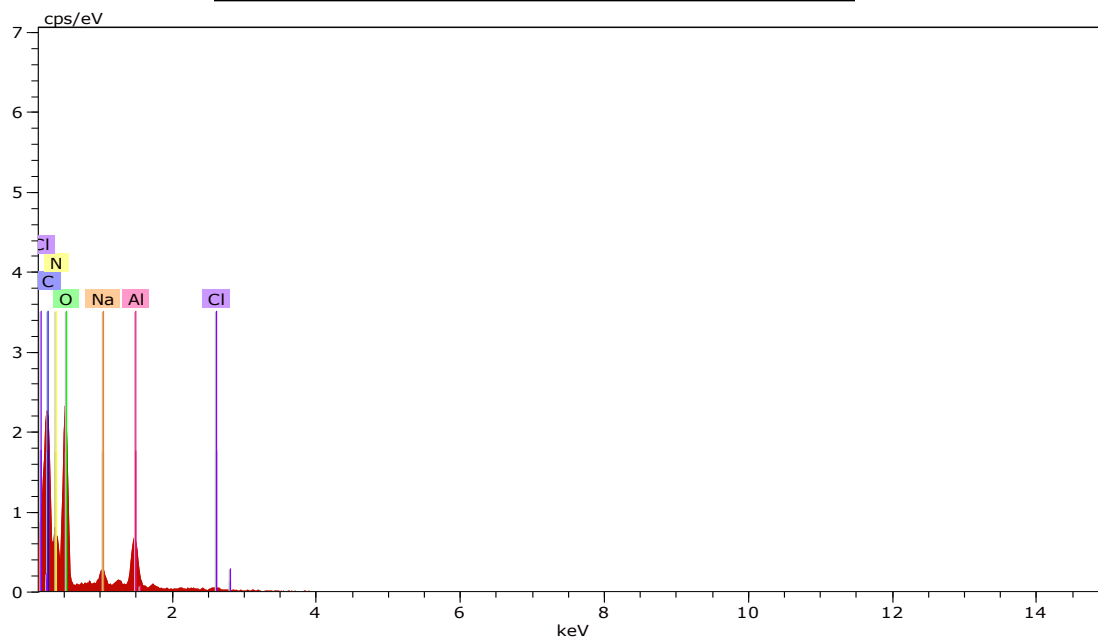
Figure 8: SEM photograph for bis glycine hydro bromide crystal

The EDX spectrum for bis glycine hydro bromide crystal is shown in Figure 9. The elemental composition present in crystal is shown in Table 3.



Table 3: Elemental composition for bis glycine hydro bromide crystal

| Elements | Bis glycine hydro bromide | |
|----------|---------------------------|----------|
| | Atomic % | Weight % |
| C | 33.74 | 28.10 |
| N | 24.49 | 23.39 |
| O | 39.09 | 43.36 |

*Figure 9: EDX chart for bis glycine hydro bromide crystal*

This study reveals that C, N and O elements are present in the title crystal

4.6. Antimicrobial activity study

The glycine and bis glycine hydro bromide crystals were tested against *Bacillus subtilis*, *Micrococcus*, *Salmonella typhi* and *Pseudomonas* organisms to analyze the antimicrobial activity by disc diffusion method. The photographic view of bacterial screening for parent and its complex crystals with 50 μ g/ml and 100 μ g /l concentrations are shown in figure.10a and 10b respectively. The measured diameter zone of inhibition of these microorganisms is given in Table 4.



Figure 10a: Photographic view showing inhibition region of four different micro-organisms at 50 μ g/ml and 100 μ g/l concentrations against glycine crystal



Figure 10b: Photographic view showing inhibition region of four different micro-organisms at 50µg/ml and 100 µg/l concentrations against bis glycine hydro bromide complex crystal

Table 4: Effective values of inhibited zone for glycine and bis glycine hydro bromide crystal

| S. No. | Micro-organisms | Zone of inhibition for glycine | | Zone of inhibition for bis glycine hydro bromide crystal | |
|--------|-------------------|--------------------------------|-------------|--|-------------|
| | | 50 µl (mm) | 100 µl (mm) | 50 µl (mm) | 100 µl (mm) |
| 1. | Bacillus subtilis | NIL | NIL | NIL | NIL |
| 2. | Micrococcus | NIL | 4 | NIL | NIL |
| 3. | Salmonella typhi | NIL | NIL | NIL | NIL |
| 4. | Pseudomonas | NIL | NIL | NIL | NIL |

*NIL- No antimicrobial activity; mm- zone of inhibition

From the Table 4, it is clear that glycine and its complex crystals have no antimicrobial activity for four different test bacterias. But, the glycine crystal shows the effective zone of inhibition (4 mm) for Micrococcus organism in 100 µl concentration.

5. Conclusion

The bis glycine hydro bromide crystal was grown at room temperature by the slow evaporation technique. The unit cell parameters and space group were assessed by single-crystal X-ray diffraction technique. This study reveals that the title crystal structure exists in the zwitterion as well as cationic forms and has orthorhombic crystal system with the space group $P2_12_12_1$. The dislocation density and the average crystalline size of grown crystal was found from the PXRD patterns and the peaks were indexed using the INDX software. Further, the presence of various functional groups and elements were verified using FT-IR and FT-Raman spectroscopy and Energy dispersive X-ray studies. The SEM analyzes shows that the title crystal has smooth surface and well defined shape with small voids and porous. Also, the optical band gap was determined as 5.6 eV by UV- Visible spectroscopy technique. The grown parent and its complex crystals were involved in an antibacterial activity against certain four micro-organisms by disc diffusion method. This study revealed that the pure glycine and bis glycine hydro bromide complex crystals have no bacterial screening effect.

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