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## Research Article Vibrational, Optical and Antimicrobial Activity Studies on Diglycine Perchlorate Single Crystal

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### Abstract

**Background and Objective:** The glycine compound with inorganic acid play an extensive roles in the nonlinear optical applications. The main objective of the present work was to observe the growth and characterization of the title crystal using single crystal XRD, PXRD, FT-IR and FT-Raman, UV-Visible spectroscopy, SEM with EDX and antimicrobial activity studies. **Materials and Methods:** Glycine, perchloric acid and deionized water used for the crystallization, the single crystals were obtained at room temperature and the antimicrobial activity of title crystal was observed against 5 different kinds of micro-organisms. **Results:** The crystal system, lattice parameters and space group were determined and are found to be in good agreement with the already reported values. The crystalline nature and various functional groups present in the crystal were analyzed. The optical band gap was determined as 5.4 eV and morphology with the elemental analysis have been performed. The antimicrobial activity was established against the 5 different micro-organisms. **Conclusion:** The title compound belongs to triclinic crystal system with the space group Pī. The FT-IR, FT- Raman spectroscopic techniques elucidate the several functional groups present in the molecule. The UV-visible spectroscopy study revealed that the grown crystal has high transparency in the entire visible region. The morphology and elemental analysis have also been performed. The antibacterial activity does not appear against the PAO-1, MRSA, S.epi, C.Vio and S.Mar micro-organisms.

Key words: Diglycine perchlorate, XRD, IR, raman, UV, screening effect, symmetry

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Competing Interest: The authors have declared that no competing interest exists.

Data Availability: All relevant data are within the paper and its supporting information files.

#### INTRODUCTION

Glycine is the simplest and optically inactive amino acid<sup>1</sup>. It has no asymmetric carbon atom<sup>2</sup>. Due to the zwitterionic nature of glycine, it is capable of forming compounds with charged and uncharged chemical composites<sup>3,4</sup>. This zwitterionic nature helps to increase the physical properties, which thus making them ideal candidates for nonlinear optical applications<sup>5</sup>. In recent years, efforts have been made to crystallize the glycine complexes with inorganic acids in order to improve the chemical stability, linear and nonlinear optical properties<sup>6,7</sup>. Recently, Muthuselvi *et al.*<sup>8,9</sup> reported the spectral and antimicrobial activity studies on bis glycine hydro bromide and glycinium dihydrogen phosphate complex crystals. In the continuation of this previous work, the glycine mixes with the perchloric acid, leading to the formation of diglycine perchlorate (GlyH.Gly.ClO<sub>4</sub>) and this crystal structure was already reported by Ghazaryan *et al.*<sup>10</sup>. Motivated by the applications of the diglycine perchlorate single crystal in materials science, an attempt has been made on the growth of diglycine perchlorate crystal by slow evaporation method. The grown crystal is characterized by single crystal XRD, powder XRD, FT-IR, FT-Raman, UV-Visible spectroscopy, SEM analysis. These results are discussed and with EDX summarized in this present work. Apart from these, the antibacterial activity study seems to be enhanced because none of them were reported to this property for this title compound.

#### **MATERIALS AND METHODS**

**Study area:** The crystal was grown in the month of April, 2018 at the Research Department of Physics, Devanga Arts College, Aruppukkottai. Here all the data were collected from the various places in the month of August-September, 2019.

**Research chemicals:** The raw materials used for the crystallization of title compound are glycine, perchloric acid and deionized water and which were purchased from Sigma Aldrich Company, India.

**Research procedure:** The single crystal of diglycine perchlorate is obtained from slow evaporation technique. Initially an equimolar ratio (1:1) of glycine and perchloric acid were dissolved in deionized water. This solution was stirred well for 1 h and it was filtered using high quality filter paper. The filtered solution was poured into the



Fig. 1: Grown crystal of diglycine perchlorate

petri dish. Now the petri dish was tightly closed with thick filter paper due to minimize the rate of evaporation at room temperature. After a period of 1 week, transparent block-shaped crystals were harvested and the photographic view of grown crystal is depicted in Fig. 1.

#### **Data collection**

**Single and powder crystal XRD analysis:** The single crystals of diglycine perchlorate were grown by the slow evaporation technique and the good quality single crystal was selected to carry out the single crystal X-ray diffraction using Bruker SMART APEX CCD diffractometer with MoK $\alpha$  radiation ( $\lambda = 0.71073$  Å). Data was collected from SAIF, IIT Madras, Chennai. The powder diffraction pattern was recorded at Alagappa University, Karaikudi using XPERT-PRO X-ray diffractometer with CuK $\alpha$  ( $\lambda = 1.54060$  Å) radiation.

**Spectral data analysis:** Using SHIMADZU FT-IR spectrometer, FT-IR vibrational spectrum was recorded in the range 4000-400 cm<sup>-1</sup>. Also, the FT-Raman spectrum was recorded using the BRUKER: RFS 27 Raman spectrometer in the wavenumber range 4000-400 cm<sup>-1</sup>. These spectral data were taken from SAIF, IIT Madras, Chennai. The optical absorption spectrum of diglycine perchlorate crystal has been recorded with SHIMADZU-UV1800 double beam spectrometer in the wavelength range 200-1100 nm in steps of 1 nm at V.H.N.S.N. College, Virudhunagar.

**SEM with EDX analysis:** The surface morphology and elemental analysis has been carried out by CARLZEISS EVO18 scanning electron microscope. This data was taken from the Kalasalingam University, Krishnankoil.

**Antimicrobial study:** The antimicrobial activity of title crystal was confirmed against 5 different kinds of micro-organisms (PAO-1, MRSA, S. epi, C. Vio and S. mar) using the disc diffusion method which is analyzed at Kaliswari College, Sivakasi.

**Statistical analysis:** The origin software was used in powder XRD, FT-IR, FT-Raman and UV-Visible spectroscopic data analysis.

#### **RESULTS AND DISCUSSION**

The single crystal XRD values are tabulated in Table 1 and compared with the already reported values<sup>10</sup>. The molecular structure of diglycine perchlorate crystal is shown in Fig. 2. In addition to single crystal XRD analysis, powder diffraction data was collected for diglycine perchlorate crystal. The powder XRD pattern of the title crystal is shown in Fig. 3. The experimentally recorded FT-IR and FT-Raman spectra of title compound are shown in Fig. 4 and 5, respectively. The detailed wavenumber assignment for the title crystal is presented in Table 2. The symmetry of perchlorate anion is shown in Table 3. The experimentally recorded absorbance spectrum and determination of energy band gap graph is shown in Fig. 6 and 7, respectively. The SEM image is represented in Fig. 8. The EDX spectrum for diglycine perchlorate crystal is exposed in Fig. 9. The elemental composition present in diglycine perchlorate crystal is shown in Table 4. The photographic view of bacterial screening for title crystal with 50 and 100 µL concentrations is shown in Fig. 10. The measured diameter zone of inhibition of the micro-organisms is given in Table 5.

**Single crystal x-ray diffraction:** In the crystal structure of diglycine perchlorate, the glycine molecule I exists in the zwitterionic form  $NH_3^+CH_2COO^-$  and the glycine molecule II exists in the cationic form  $NH_3^+CH_2COOH$ . Here, a proton of perchloric acid is liberated and protonated with the one glycine  $NH_2$  group which then becomes as glycinium cation and perchlorate anion. Also, this study confirms the grown crystal crystallizes in the triclinic system with space group Pī.

**Powder XRD analysis:** The appearance of sharp and strong peaks established the good crystallinity nature of the grown crystal. The characteristic peak of this compound has appeared at around 29.69°. Using INDX software, the PXRD patterns are indexed. The average crystalline size is found to be as 44 nm for title crystal using this Eq:

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



Fig. 2: Molecular structure of diglycine perchlorate crystal



Fig. 3: Diffraction patterns for diglycine perchlorate crystal

Table 1: Crystallographic data of diglycine perchlorate crystal

| ,                    | ÷, ,                              |                                   |
|----------------------|-----------------------------------|-----------------------------------|
| Lattice parameters   | Present study                     | Already reported <sup>10</sup>    |
| Compound name        | Diglycine perchlorate             | Diglycine perchlorate             |
| Empirical formula    | $C_4H_{11}N_2O_4^+ \cdot CIO_4^-$ | $C_4H_{11}N_2O_4^+ \cdot CIO_4^-$ |
| Molecular weight     | 250.60                            | 250.60                            |
| Unit cell dimensions | a = 8.685 (3) (Å)                 | a = 8.700 (2) (Å)                 |
|                      | b = 14.840 (2) (Å)                | b = 14.842 (2) (Å)                |
|                      | c = 19.402 (3) (Å)                | c = 19.396 (2) (Å)                |
|                      | α = 98.739 (5)°                   | $\alpha = 98.748(7)^{\circ}$      |
|                      | β = 93.104 (9)°                   | $\beta = 93.056(9)^{\circ}$       |
|                      | $\gamma = 106.048 (7)^{\circ}$    | $\gamma = 106.053(9)^{\circ}$     |
| Volume               | 2375.6 (8) (Å) <sup>3</sup>       | 2366.8(7) (Å) <sup>3</sup>        |
| Crystal system       | Triclinic                         | Triclinic                         |
| Space group          | Pī                                | Pī                                |

The dislocation density can be calculated from the Eq:

$$\delta = \frac{1}{D^2} m^2 = 5.17 \times 10^{14} m^2$$

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Fig. 4: FT-IR spectrum of diglycine perchlorate crystal



Fig. 5: FT-Raman spectrum of diglycine perchlorate crystal

**Vibrational analysis:** The crystal structure of diglycine perchlorate exists both in the zwitterionic and cationic forms. The zwitterionic form of glycine molecule has  $[NH_3]^+$ , COO<sup>-</sup> and CH<sub>2</sub> functional groups and cationic form has  $[NH_3]^+$ (cation), COOH, CH<sub>2</sub> and ClO<sub>4</sub><sup>-</sup> (anion) functional groups.

**Vibrations of -[NH<sub>3</sub>]<sup>+</sup> group:** The antisymmetric and symmetric stretching modes of -[NH<sub>3</sub>]<sup>+</sup> group are found in the range of 3200 and 2800 cm<sup>-1</sup>, respectively<sup>11</sup>. In the present study, a strong broad band at 3171 cm<sup>-1</sup> in IR and a weak band at 3141 cm<sup>-1</sup> in Raman spectra is identified and assigned to the  $v_{as}$ -[NH<sub>3</sub>]<sup>+</sup> mode. Also  $v_s$ -[NH<sub>3</sub>]<sup>+</sup> mode is attributed at 2971, 2916 and 2880 cm<sup>-1</sup> in Raman spectra. The



Fig. 6: Absorbance spectrum for diglycine perchlorate crystal



Fig. 7: Optical band gap for diglycine perchlorate crystal

antisymmetric and symmetric deformation modes of -[NH<sub>3</sub>]<sup>+</sup> group are normally expected to fall in the region of 1625-1550 and 1550-1505 cm<sup>-1</sup>, respectively<sup>11,12</sup>. The  $\delta_{as}$ -[NH<sub>3</sub>]<sup>+</sup> wavenumber is assigned at 1626 cm<sup>-1</sup> in IR and at 1668 cm<sup>-1</sup> in Raman spectra. Also, the  $\delta_{s}$ -[NH<sub>3</sub>]<sup>+</sup> band is attributed at 1595, 1541 cm<sup>-1</sup> in IR and at 1568 cm<sup>-1</sup> in Raman spectra study. The broad band centered at 3000 cm<sup>-1</sup> in IR spectrum is attributed to the presence of extensive three dimensional hydrogen bonding network that exists in the crystal. Due to the presence of hydrogen bonding modes of -[NH<sub>3</sub>]<sup>+</sup> group are deviated from the free ion.



#### Fig. 8: SEM photograph for diglycine perchlorate crystal

Table 2: Wavenumber assignments for diglycine perchlorate crystal in FT-IR and FT-Raman spectra

| FT-IR ( $\overline{\nu}$ cm <sup>-1</sup> ) | FT-Raman ( $\overline{v}$ cm <sup>-1</sup> ) | Assignment   |
|---|--|--|
| 3431 (s)                                    | -  | v (O-H) <sub>Water</sub>   |
| 3171 (s, br)                                | 3141 (w)                                     | $\nu_{as}$ [NH <sub>3</sub> ] <sup>+</sup>   |
| -   | 3006 (s)                                     | v (O-H)  |
| -   | 2971 (s)                                     | $v_{s} [NH_{3}]^{+}, v_{as} (CH_{2})$  |
| -   | 2916 (w)                                     | ν <sub>s</sub> [NH <sub>3</sub> ] <sup>+</sup> , ν <sub>s</sub> (CH <sub>2</sub> ) |
| -   | 2880 (m)                                     | $v_{s} [NH_{3}]^{+}$   |
| 1715 (w)                                    | -  | v <sub>as</sub> (C=O)  |
| 1626 (s, br)                                | -  | δ (O-H) <sub>Water</sub>   |
| -   | 1668 (m)                                     | ν <sub>s</sub> (C=O)   |
| 1595 (s)                                    | 1568 (m)                                     | $\delta_{as}$ [NH <sub>3</sub> ] <sup>+</sup> , $\nu_{as}$ (COO <sup>-</sup> )     |
| 1541 (s)                                    | -  | $\delta_s [NH_3]^+$  |
| 1520 (s)                                    | 1511 (m)                                     | $\delta_s [NH_3]^+$  |
| 1451 (s)                                    | 1455 (m)                                     | ρ (CH <sub>2</sub> ), β (O-H)  |
| -   | 1438 (m)                                     | β (O-H)  |
| 1416 (s)                                    | 1410 (s)                                     | β (O-H)  |
| 1331 (s)                                    | 1324 (s)                                     | ω (CH <sub>2</sub> ), ν <sub>s</sub> (COO <sup>-</sup> )                           |
| 1115 (m)                                    | -  | $v_{as}$ [CIO <sub>4</sub> ] <sup>-</sup>  |
| -   | 1138 (w)                                     | ν <sub>as</sub> [CIO <sub>4</sub> ] <sup>-</sup> , υ (C-N)                         |
| 1032 (m)                                    | 1034 (m)                                     | ν <sub>as</sub> [ClO <sub>4</sub> ] <sup>-</sup> , υ (C-C)                         |
| 907 (m)                                     | -  | ν <sub>s</sub> [CIO <sub>4</sub> ] <sup>-</sup>                                    |
| 895 (m)                                     | 892 (s)                                      | γ (O-H), υ (C-C)   |
| 696 (m)                                     | 695 (m)                                      | ρ (COO <sup>_</sup> )  |
| 673 (w)                                     | -  | $\delta_{as} [CIO_4]^-$  |
| 626 (w)                                     | -  | $\delta_{as}$ [CIO <sub>4</sub> ] <sup>-</sup>                                     |
| 606 (m)                                     | 599 (m)                                      | $\delta_{as}$ [CIO <sub>4</sub> ] <sup>-</sup> , $\rho$ (COO <sup>-</sup> )        |
| 505 (m)                                     | -  | ρ (COO <sup>_</sup> )  |
| -   | 496 (m)                                      | δ <sub>s</sub> [CIO <sub>4</sub> ] <sup>-</sup>                                    |
| -   | 487 (m)                                      | $\delta_s [CIO_4]^-$   |

w: Weak, s: Strong, m: Medium, v: Stretching; v<sub>s</sub>: Symmetric stretching, v<sub>a</sub>: Anti symmetric stretching,  $\delta$ : bending,  $\delta_s$ : Symmetric bending,  $\delta_{as}$ : Antisymmetric bending,  $\gamma$ : Out-of-plane bending,  $\beta$ : In-plane bending,  $\rho$ : Scissoring,  $\omega$ : Wagging

**Vibrations of [ClO<sub>4</sub>]<sup>–</sup> group:** The IR spectrum of perchlorate anion is already reported by Chen *et al.*<sup>13</sup>, Wittenkeller *et al.*<sup>14</sup>, Muthuselvi *et al.*<sup>15</sup>, Siva *et al.*<sup>16</sup>, Mary *et al.*<sup>17</sup> and Petrosyan<sup>18</sup>. In free state, the perchlorate ion has  $T_d$  symmetry with its vibrational modes distributed as:

| [able 3: Vibrational distribution of [ClO <sub>4</sub> ] <sup>-</sup> | ion |
|---|-----|
|---|-----|

| T <sub>d</sub> (cm <sup>-1</sup> ) | C <sub>2v</sub> (cm <sup>-1</sup> )                   | Present study (cm <sup>-1</sup> ) |
|------------------------------------|---|-----------------------------------|
| A <sub>1</sub> (928)               | A <sub>1</sub> (928)                                  | A <sub>1</sub> (907)              |
| E (459)                            | A <sub>1</sub> (460)                                  | A <sub>1</sub> (496)              |
|                                    | A <sub>2</sub> (440)                                  | A <sub>2</sub> (487)              |
| F <sub>2</sub> (1119)              | A <sub>1</sub> (1038)                                 | A <sub>1</sub> (1032)             |
|                                    | B <sub>1</sub> (1125)                                 | B <sub>1</sub> (1115)             |
|                                    | B <sub>2</sub> (1170)                                 | B <sub>2</sub> (1138)             |
| F <sub>2</sub> (625)               | A <sub>1</sub> (635)                                  | A <sub>1</sub> (673)              |
|                                    | B <sub>1</sub> (617)                                  | B <sub>1</sub> (606)              |
|                                    | B <sub>2</sub> (623)                                  | B <sub>2</sub> (626)              |
| Table 4: Elemental                 | composition for diglycine perch<br>Diglycine perchlor | lorate crystal                    |
|                                    |   |                                   |
| Elements                           | Atomic (%)  | Weight (%)                        |
| С                                  | 33.9  | 28.4                              |
| Ν                                  | 20.8  | 20.3                              |

#### $G = A_1 + E + 2F_2$

44.8

0.5

50.0

1.3

where,  $A_1$  and E species are Raman active only while the two  $F_2$  species are both IR and Raman active. These modes are expected to occur at 928, 459, 1119 and 625 cm<sup>-1</sup>, respectively for the perchlorate ion<sup>19</sup>. The perchlorate anion oxygen atoms form the hydrogen bond with the -[NH<sub>3</sub>]<sup>+</sup> group of one glycine molecule which reduces the  $T_d$  symmetry of perchlorate anion to  $C_{2v}$  symmetry. In this case, the vibrational modes are distributed as:

#### $\Gamma = 4A_1 + A_2 + 2B_1 + 2B_2$

The F<sub>2</sub> (v<sub>as</sub>) species splits into 3 appearing at 1038 (A<sub>1</sub>), 1125 (B<sub>1</sub>) and 1170 (B<sub>2</sub>) cm<sup>-1</sup>. The A<sub>1</sub> (v<sub>s</sub>) species occurs at 928 cm<sup>-1</sup> while  $\delta_{as}$  (F<sub>2</sub>) wave number occurs at 635 (A<sub>1</sub>), 617 (B<sub>1</sub>) and 623 (B<sub>2</sub>) cm<sup>-1</sup>. The  $\delta_{sym}$  species (E) breaks up into

0

Cl

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Fig. 9: EDX spectrum for diglycine perchlorate crystal



Fig. 10: Photographic view showing inhibition region of 5 different micro-organisms at 50 and 100 µL concentrations against diglycine perchlorate crystal

| Micro-organisms                             | Zone of inhibition for diglycine perchlorate crystal |             |
|---|--|-------------|
|   |  | 100 μL (mm) |
| Polyphosphate-accumulating organisms        | NIL  | NIL         |
| Methicillin-resistant Staphylococcus aureus | NIL  | NIL         |
| Staphylococcus epidermidis                  | NIL  | NIL         |
| Chromobacterium violaceum                   | NIL  | NIL         |
| Serratia marcescens                         | NIL  | NIL         |

Table 5: Effective values of inhibited zone for diglycine perchlorate crystal

NIL: No antimicrobial activity, mm: Zone of inhibition

2 bands at nearly 460 cm<sup>-1</sup> (A<sub>1</sub>, A<sub>2</sub>). Here The A<sub>2</sub> species is only Raman active and the all other species are both IR and Raman active<sup>20</sup>.

In the present work, the antisymmetric stretching mode of  $[CIO_4]^-$  ion is assigned at 1115 and 1032 cm<sup>-1</sup> in IR spectrum. The same mode is identified at 1138, 1034 cm<sup>-1</sup> in Raman spectrum. The symmetric stretching mode of  $[CIO_4]^-$  anion is assigned at 907 cm<sup>-1</sup> in the IR spectrum only.

The antisymmetric bending mode is observed at 673 (A<sub>1</sub>), 606 (B<sub>1</sub>) and 626 (B<sub>2</sub>) cm<sup>-1</sup> in IR spectra. The symmetric bending mode is observed at 496, 487 cm<sup>-1</sup> in Raman spectrum only for the title crystal. The assignments for this perchlorate anion are exactly matched with earlier reported values<sup>19,20</sup> which confirm the symmetry of perchlorate anion is C<sub>2v</sub> not T<sub>d</sub> and it is clearly identified from the Table 3.

**Vibrations of CH<sub>2</sub> group:** Normally, the CH<sub>2</sub> antisymmetric and symmetric stretching vibrations can exist in the region of 3000-2900 and 2900-2800 cm<sup>-1</sup>, respectively<sup>21-23</sup>. In the present study  $v_{as}$ (CH<sub>2</sub>) and  $v_{s}$ (CH<sub>2</sub>) modes are attributed at 2971 and 2880 cm<sup>-1</sup> in the Raman spectrum only. The CH<sub>2</sub> scissoring, wagging and twisting modes fall in the range 1482-1437, 1390-1180 and 730-720 cm<sup>-1</sup>, respectively<sup>24</sup>. In the present study, the absorption bands appeared at 1451 cm<sup>-1</sup> in IR and at 1455 cm<sup>-1</sup> in Raman spectra is assigned to CH<sub>2</sub> scissoring mode. Also, CH<sub>2</sub> wagging mode is attributed at 1331 cm<sup>-1</sup> (IR), 1324 cm<sup>-1</sup> (Raman). The twisting and rocking modes are not acknowledged for the title compound.

Vibrations of C=O, C-O and O-H groups: The C=O group has IR band in the region 1720-1680 and 1680-1640  $cm^{-1}$  for antisymmetric and symmetric stretching modes respectively<sup>25</sup>. The band occurs at 1715 cm<sup>-1</sup> in IR is allocated to  $v_{as}$  (C=O) mode. Also, bands occurring at 1668 cm<sup>-1</sup> in Raman spectra is assigned to the  $v_s$ (C=O) mode. The O-H stretch from CO-OH group is identified<sup>25</sup> at 3065-2826 cm<sup>-1</sup>. For the title compound, this mode is attributed at 3006 cm<sup>-1</sup> in Raman spectrum only. The in-plane and out-of-plane bending wavenumbers of O-H group appears in the region between 1440-1395 and 960-875 cm<sup>-1</sup>, respectively<sup>25,26</sup>. In the present work,  $\beta$ (O-H) mode is observed at 1451, 1416 cm<sup>-1</sup> in IR and at 1455, 1438, 1410 cm<sup>-1</sup> in Raman spectra, respectively. Also  $\gamma$  (O-H) mode is attributed at 895, 892 cm<sup>-1</sup> in both spectra of title compound. These modes of assignments confirm the cationic form of glycine molecule.

**Vibration of COO<sup>-</sup> group:** The ionized carboxylic COO<sup>-</sup> group provides the antisymmetric and symmetric stretching modes

in the regions 1600-1580 cm<sup>-1</sup> and at 1400-1280 cm<sup>-1</sup>, respectively<sup>27</sup>. The  $v_{as}$ (COO<sup>-</sup>) mode is attributed as a strong intensity band at 1595 cm<sup>-1</sup> in IR and as a medium band at 1568 cm<sup>-1</sup> in Raman spectra for the title compound. Also, the symmetric stretching mode  $v_s$ (COO<sup>-</sup>) for the same group is identified at 1331 cm<sup>-1</sup> in IR and at 1324 cm<sup>-1</sup> in Raman spectra. The scissoring, wagging and rocking deformation modes of COO<sup>-</sup> ionized carboxylic group are normally expected at 665, 577 and 502 cm<sup>-1</sup>, respectively<sup>27</sup>. For the title compound, these modes are assigned at 696, 606, 505 cm<sup>-1</sup> in IR and at 695, 599 cm<sup>-1</sup> in Raman spectra, respectively. These bands are assigned to the carbonyl group of glycine molecule in zwitterionic form.

**Vibrations of other groups:** The C-C stretching and bending modes normally fall in the<sup>28</sup> range 1117-870 cm<sup>-1</sup>. The C-N absorption bands for aliphatic amines appear in the region<sup>28</sup> of 1250-1020 cm<sup>-1</sup>. In the present study, the bands identified at 1032, 895 cm<sup>-1</sup> in IR spectrum and at1034, 892 cm<sup>-1</sup> in Raman spectrum is assigned to the v (C-C) mode of title compound. Also, the v (C-N) mode is attributed at 1138 cm<sup>-1</sup> in Raman spectrum.

**Vibrations of water molecule:** The strong peak that occurred at 3431 cm<sup>-1</sup> in the IR spectrum is due to absorption of water molecule during KBr pellet preparation. It is assigned to the symmetric stretching mode of water. The medium band at 1626 cm<sup>-1</sup> is assigned to the bending mode of water molecule.

**Optical study:** The lower cut-off wavelength is found at 245 nm. The title crystal has 100% transmittance in the entire visible region which makes usefulness of this material in optical application. The Tauc's relation  $(\alpha h \nu)^2 = A(h\nu - E_g)$  is used to determine the energy gap  $E_g$  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 diglycine perchlorate crystal. From the Fig. 7,  $E_g$  is found as 5.4 eV and this value reveals that the grown crystal is a typical of dielectric material.

**SEM with EDX analysis:** The SEM images with 2 different magnifications revealed that the grown crystal has the well-defined shape. The EDX study confirms the presence of C, N, O and CI elements in the diglycine perchlorate crystal.

**Antimicrobial activity study:** The polyphosphateaccumulating organisms, Methicillin-resistant *Staphylococcus aureus, Staphylococcus epidermidis,*  *Chromobacterium violaceum* and *Serratia marcescens* micro-organisms were tested to analyze the antimicrobial activity of diglycine perchlorate crystal by disc diffusion method. The diglycine perchlorate single crystal has no antimicrobial activity against 5 different test bacteria.

#### CONCLUSION

The diglycine perchlorate single crystals have been crystallized at room temperature using the slow evaporation technique. The single crystal X-ray data suggests that the title crystal has triclinic crystal system with the space group P1. The PXRD peaks were indexed using the INDX software and the average crystalline size of grown crystal was found to be as 44 nm. Further, the vibrational assignments of bands in the FT-IR and FT-Raman spectra were performed for diglycine perchlorate crystal. Due to the extensive intermolecular hydrogen bonding and coordination of the perchlorate anion, the  $T_d$  symmetry of the anion is reduced to  $C_{2v}$  symmetry. Using the UV-Visible spectroscopy analysis, the optical band gap was determined as 5.4 eV. The SEM analysis shows that the title crystal has well defined shape. The EDX study confirms the true composition of elements present in the diglycine perchlorate crystal. The antibacterial activity study revealed that the diglycine perchlorate complex crystal has no bacterial screening effect against certain 5 different micro-organisms by disc diffusion method.

#### SIGNIFICANCE STATEMENTS

This study realizes the semi-organic glycine derivative compound with inorganic acid that can play the extensive roles in the nonlinear optical applications. This study will help the researcher to develop and increase the physical property of the material in the field of materials science. In order to improve the chemical stability, linear and nonlinear optical properties, a new attempt was made on the growth of diglycine perchlorate single crystal by slow evaporation method. Apart from the structural, vibrational and optical studies, the morphology and the antibacterial activity analysis appear to be enhanced in the present study.

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