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Synthesis and Growth of New Nonlinear Optical Material for Technological Applications

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Abstract: ***New nonlinear optical single crystal of D-Phenylglycinium bromide (DPGB) was grown by slow evaporation solution growth technique and characterization studies were carried out for the first time. The structure of the grown crystal was elucidated using single crystal X-ray diffraction. EDAX analysis was carried out to confirm the presence of constituent elements in the material. The presence of various functional groups were identified by FT-IR spectral analysis. Optical transmission spectra revealed the optical properties of the grown crystal. The thermal stability of the title crystal was investigated using Thermogravimetric analysis. The second harmonic generation efficiency of the material was tested by Kurtz-Perry powder technique.***

Keywords: Crystal growth ; Characterization ; X-ray diffraction ; Thermal analysis ; Nonlinear optical materials.

I. INTRODUCTION

Organic molecules able to manipulate photonic signals efficiently are of importance in technologies such as optical computing and dynamic image processing [1,2]. Glycine is the simplest form of amino acid which reacts with other inorganic compounds to give a good mechanical and thermal stability. Phenylglycine derivatives play an important role in the synthesis of antitumor drugs and other pharmacological applications [3,4]. Phenylglycine was reported as a delivery tool for improving l-dopa absorption [5] and also found to have anti-inflammatory activity [6]. The crystal structures of D-Phenylglycine hydrochloride [7], D-Phenylglycinium nitrate [8], D-Phenylglycinium perchlorate [9], were reported. In addition to the reported works in the literature, a new nonlinear optical crystal of D-Phenylglycinium bromide was grown by us and its crystal structure was reported [10]. The grown crystal was subjected to different characterization studies such as single crystal X-ray diffraction, EDAX analysis, Fourier transform Infrared (FT-IR) spectral analysis, UV-Visible absorption, Thermal analysis and Second Harmonic Generation (SHG).

II. MATERIALS AND METHODS

The titled material was synthesized by reacting D-Phenylglycine and hydrobromic acid in the equimolar ratio 1:1 using water as solvent. The calculated amount of D-Phenylglycine was dissolved first in the deionized water and then hydrobromic acid was added to the solution slowly with continuous stirring for 5 hours. The obtained product was purified by repeated recrystallization to improve the purity of the starting material, which enhances the optical quality of the crystals. The solution was filtered in a clean vessel and optimally covered with perforated polythene sheet and kept in a constant temperature bath with a control accuracy of ±0.01ºC at 35°C. Good transparent bulk single crystals of D-Phenylglycinium bromide were harvested from the mother solution which are shown in Fig. 1.

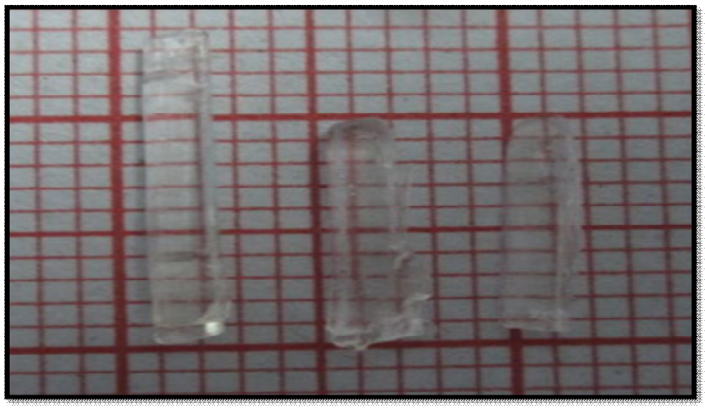

Fig.1. As grown single crystals of DPGB

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III. RESULTS AND DISCUSSION

Single crystal X-ray diffraction analysis of DPGB crystal was carried out using Bruker AXS (Kappa Apex II) X-ray diffractometer with MoKα (λ = 0.71073 Å) radiation. From the single crystal XRD analysis, it was inferred that DPGB belongs to orthorhombic crystal system with a non-centrosymmetric space group $P2_12_12_1$. The crystallographic data and the structure refinement parameters obtained by the same authors [10]

Energy dispersive spectroscopy (EDAX) is a microanalysis technique performed in combination with Quanta 200 FEG scanning electron microscope. In this investigation the title compound was subjected to EDAX analysis to confirm the presence of elemental compositions. The presence of the constituent elements in the synthesized material was confirmed by the occurrence of their respective peaks in the EDAX spectrum which is shown in Fig.2 .

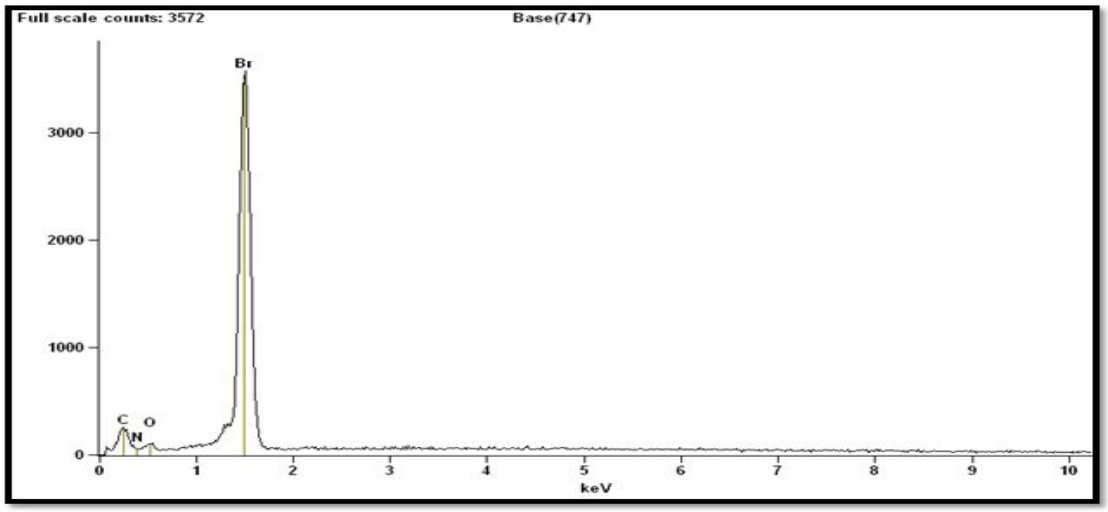

Fig.2. EDAX spectrum of DPGB

The FT-IR spectrum of the title compound was recorded between 4000 – 400 cm^{-1} by the KBr pellet technique. The resulting spectrum is shown in Fig.3. The N-H stretching vibration yield peak at 3456 cm^{-1}. The aromatic C-H stretching vibrations occurred at 3000 and 2907 cm^{-1}. The peak at 1930 cm^{-1} is attributed to combination of band of the peaks at 1018 and 921 cm^{-1} respectively. The C = O stretching vibration occurs at 1730 cm^{-1}. The N-H deformation yield its peaks at 1595 and 1558 cm^{-1}. The CH_2 bending vibrations are at 1479, 1410 and 1380 cm^{-1}. The group of peaks at 1238, 1213 and 1176 cm^{-1} corresponds to -COO- vibrations. The group of peaks below 1000 cm^{-1} is due to aromatic C-H bending vibrations. The out of plane aromatic C-H bonds were observed at 740 and 710 cm^{-1}. The NH_3^+ torsional oscillation occurs at 572 cm^{-1}. The FT-IR spectrum obtained shows the characteristic peaks of title compound.

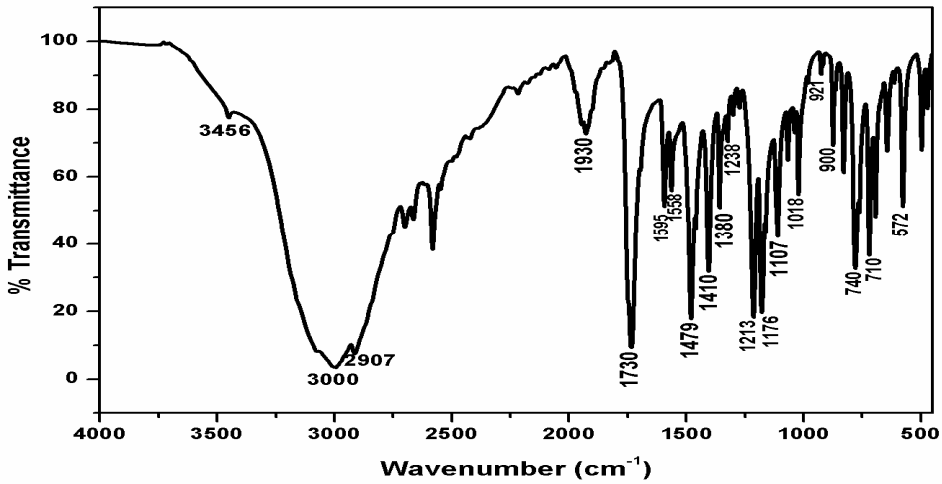

Fig.3. FT-IR spectrum of DPG

The optical absorption study on the grown crystal was carried out to record UV-Visible NIR region using VARIAN CARY 5E spectrometer in the range of 250 – 1200 nm covering the entire near UV, Visible and NIR regions. The recorded UV-Vis absorption spectrum is shown in Fig.4(a). The lower cut-off wavelength of DPGB crystal was observed at 270 nm. There is no absorption in the entire Vis-NIR range is an advantage of the essential condition for materials having NLO behaviour. Optical band gap obtained from the UV-Vis absorbance data is shown in Fig.4(b). The plot between Energy (hυ) and $(\alpha h\upsilon)^{1/2}$ is made (where α is the absorption coefficient) and the optical band gap energy [11] is found to be 4.5 eV by extrapolating the slope region (where it cuts the X-axis).

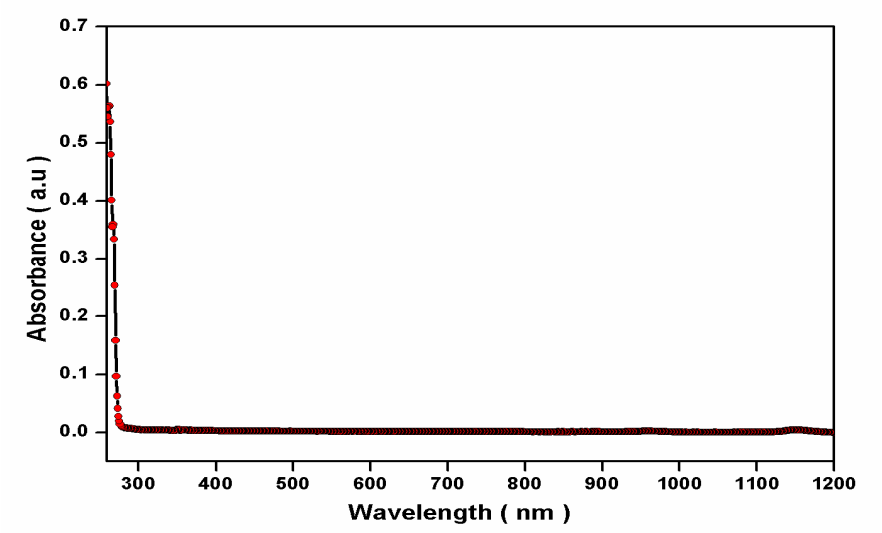

Fig.4(a). UV-Vis absorption spectrum of DPGB

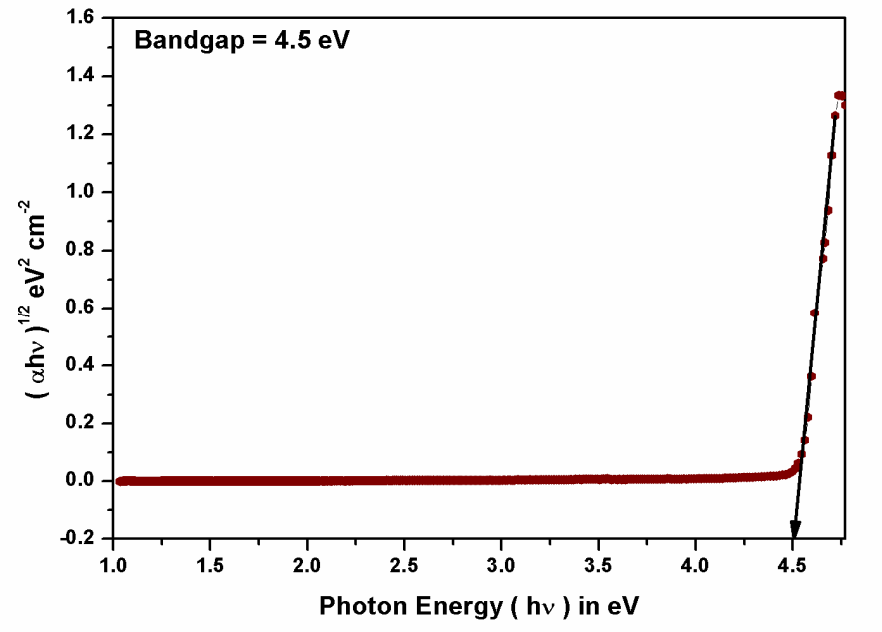

Fig.4 (b) Plot between $(\alpha h\upsilon)^{1/2}$ and hυ

The Thermogravimetric (TGA) and Differential thermal analysis (DTA) give information regarding phase transition, water of crystallization and different stages of decomposition of the crystal [12]. The thermal analyses were carried out between 40°C and 600°C at a heating rate of 10K/min in the nitrogen atmosphere. The TGA and DTA curves for the powder sample of DPGB are shown in Fig.5. From the TGA curve it is inferred that the decomposition of the title compound takes place in three stages. The initial mass of the material was taken to be 1.9150 mg and the final mass left out after the experiment was only 0.1567% (0.0030

mg). Thermogravimetric analysis shows that there is no siginificant weight loss below 200ºC, followed by a major weight loss owing to decomposition of the title compound. In DTA, there is a strong endothermic peak at 235ºC represents the melting point of the grown material. It was also verified by capillary method. Hence for NLO application of the crystal the maximum temperature is limited to 235 ºC.

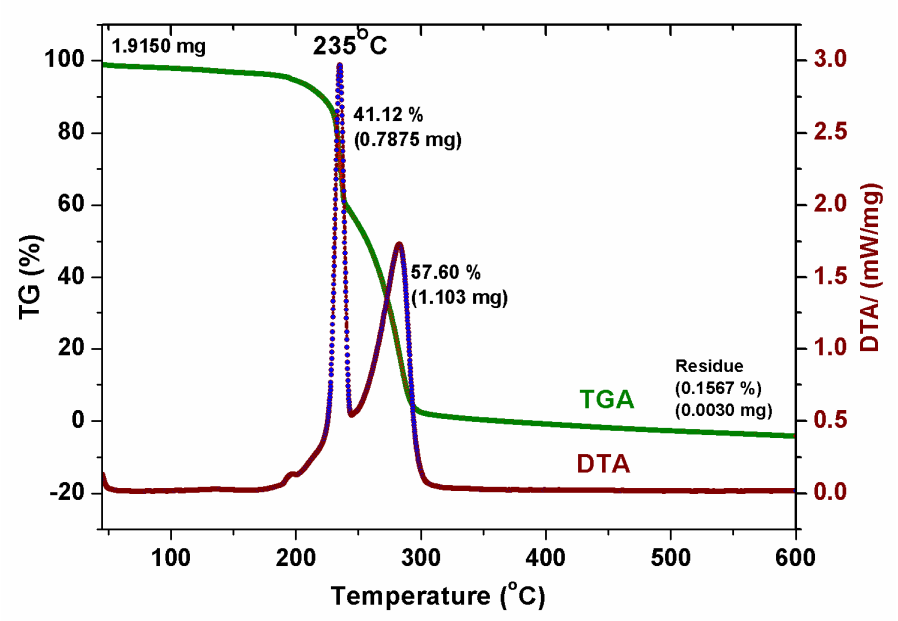

Fig.5. TG-DTA spectrum of DPGB

The SHG efficiency of the title compound was determined using Kurtz - Perry powder technique [13]. A Q-switched Nd:YAG laser beam operating at 1064 nm, with an input power of 4.1 mJ and pulse width of 8 ns with repetition rate of 10 Hz was used for this study. The output from the sample was monochromated to collect the intensity of 532 nm component. The generation of the second harmonic signal was confirmed by the emission of green light and detected by a photo multiplier tube and compared with standard KDP. It is found that SHG efficiency of DPGB is two times that of standard KDP. The second order nonlinear efficiency varies with the particle size of the powder sample [14,15].

IV. CONCLUSION

Good quality optical single crystals of D-Phenylglycinium bromide were successfully grown by solution technique. The crystal structure was elucidated using the single crystal XRD. The elements present in the synthesized material were confirmed by EDAX analysis. The functional groups were identified by FT-IR spectral analysis. The optical absorption spectral analysis reveals the crystal is transparent in the entire region with a UV cut-off wavelength of 270 nm. A sharp endothermic peak at 235ºC corresponds to the melting point of the grown material. The SHG efficiency was tested by Kurtz-Perry technique and found to be efficient compared to KDP crystal. Owing to all these properties DPGB crystal could be a promising material for the NLO application.

V. ACKNOWLEDGEMENT

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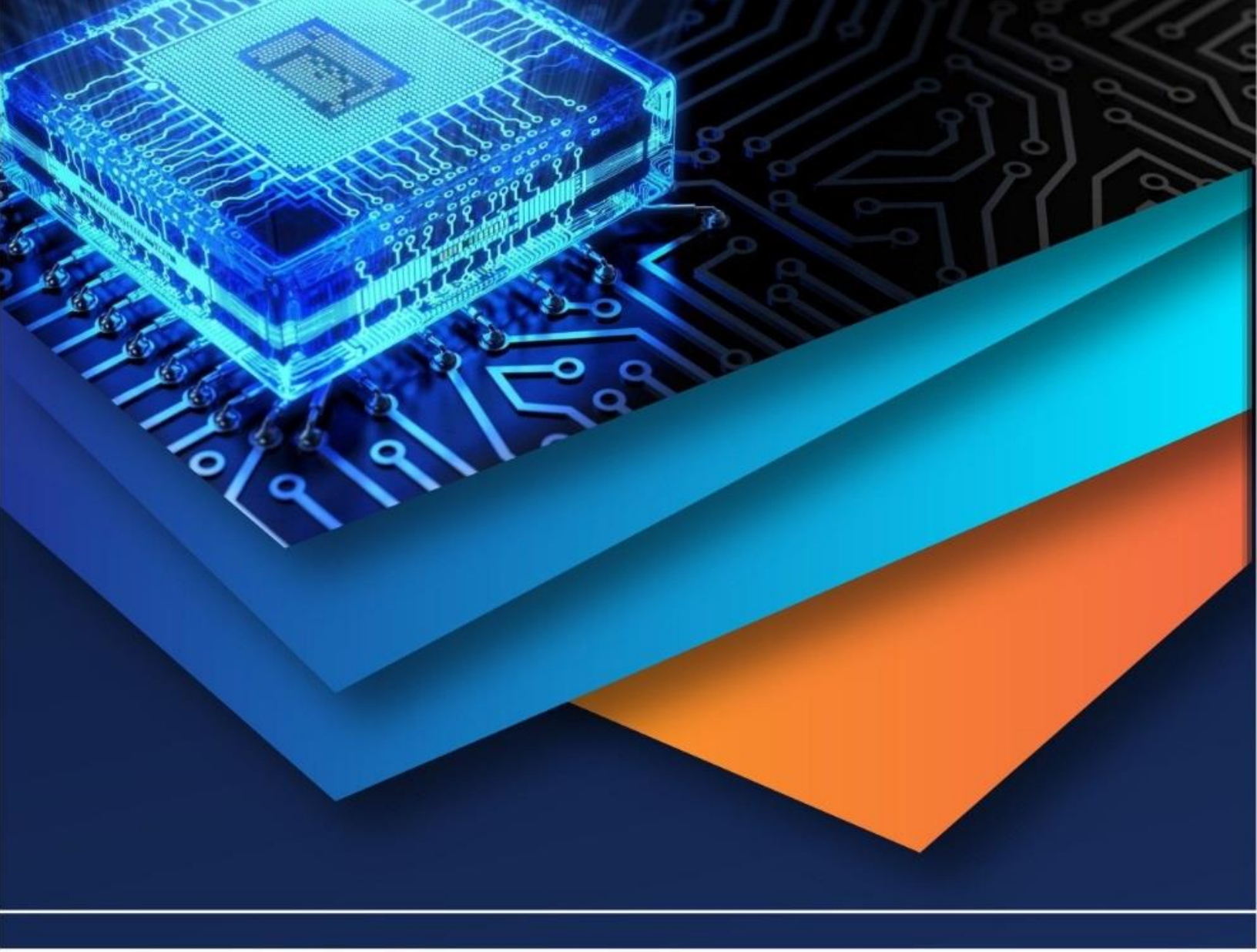

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