International Journal of Research in Science advanced Technology and management studies (IJRSTMS)

ISSN: 2459-425X • Website: www.ijrstms.com

Crystal growth, spectral, optical and thermal characterization of NLO material: 2-Aminopropionic acid (2APA)

Dr. Sai

Department of Physics, Adhi College of Engineering and Technology, Sankarapuram, Kanchipuam, Tamilnadu, India.

Abstract:

2-Aminopropionic acid (2APA) single crystals have been grown by slow evaporation solution growth technique at room temperature. The crystal structure and lattice parameters were determined for the grown crystal by single crystal X-ray diffraction studies. The bonding structure and molecular associations due to chemical reactions were analyzed and also the functional groups present in the crystals were identified using Fourier transform infrared (FTIR) and proton NMR spectrum. The UV–vis–NIR spectroscopic study revealed that the optical behavior of the grown crystal. The thermal properties were investigated by thermo gravimetric (TG) and differential thermal analysis (DTA). The optical second harmonic generation efficiency of the grown 2APA crystal was determined using Kurtz powder technique.

Keywords: Crystal growth, Crystal structure, X-ray diffraction, Optical materials.

1. INTRODUCTION

The growth of nonlinear optics (NLO) is an innovative area of research and development which will play a key role in the high technologies field of optoelectronics and photonics [1-4]. Extensive research has been focused towards materials that produce a second harmonic generation of laser light. In this connection amino acid and its derivatives possess nonlinear optical property. It is well established that donor acceptor compounds with their large differences between ground state and excited state and dipole moments as well as large transition dipole moments can exhibit large molecular second order optical nonlinearities [5-7]. Amino acids have special features such as molecular chirality, wide transparency and zwitterionic nature of the molecules. 2-Aminopropionic acid crystals have improved attention for photo induced nonlinear optical effects and increasing time of illuminations leads to considerable changes in the absorption backgrounds without changes in the spectral features [8]. In the present investigation, crystal growth, spectral, optical, thermal, and SHG efficiency of 2-Aminopropionic acid have been reported.

II. CRYSTAL GROWTH

2APA crystal was grown by slow evaporation technique using mixed solvent of doubly deionised water and methanol as a solvent. Commercially available Analytical grade (AR) 2-Aminopropionic acid was purified by repeated crystallization process before the actual growth as the quality of single crystal depends on the purity of the used materials. The growth process and the quality of the crystals significantly depend on supersaturation, appropriate selection of solvent for the growth of the material is very important in crystal growth process. Mixed solvent of doubly deionized water and methanol at 35˚ C was found to be the suitable solvent for preparing the growth solution. The super saturated solution was filtered by whatmann filter paper and allowed to evaporate slowly at room temperature over a period of one month. The grown crystal was further studied by various characterization techniques. The photographs of grown 2APA crystals are shown in Fig. 1.

International Journal of Research in Science advanced Technology and management studies (IJRSTMS)

ISSN: 2459-425X • Website: www.ijrstms.com

Fig.1. As grown crystal 2APA

III. MATERIALS CHARACTERIZATION

3.1 X-ray diffraction study

Single crystal XRD studies to confirm the cell parameters of the grown 2APA crystals, using ENRAFNONIUS CAD4-F single X-ray diffractometer with Mok$_\alpha$ (k = 0.7170 Å) radiation. Reflections from a finite number of planes were collected. The study revealed that grown 2APA crystal belongs to orthorhombic system with the following cell parameters, a = 5.714 Å, b = 11.852 Å, c = 6.131 Å and V = 415.205 (Å)3. These values have a very close agreement with reported values [9-10].

3.2 FTIR spectral analysis

The functional groups of 2APA (Fig.2) were confirmed by recording the FTIR spectrum in the range of 400–4000 cm^{-1}using BRUKER IFS – 66 V spectrometer by KBr pellet technique to confirm the presence of amino acid in the sample qualitatively. The CH stretching modes appear at 3000 cm^{-1}. The sharp intense peak at 2114 cm^{-1} is combination of NH_3 asymmetrical stretching and 1620 cm^{-1} is due to torsional oscillation. The NH_3 symmetrical stretching appears at 1519 cm^{-1}. Carboxylic stretching C=O of COO- overlapped with the NH_3 asymmetric stretching mode. The sharp peaks at 1364 and 1463 cm^{-1} are due to CH_2 bending. The peaks at 1307 and 1237 cm^{-1} are C-COO vibration modes.

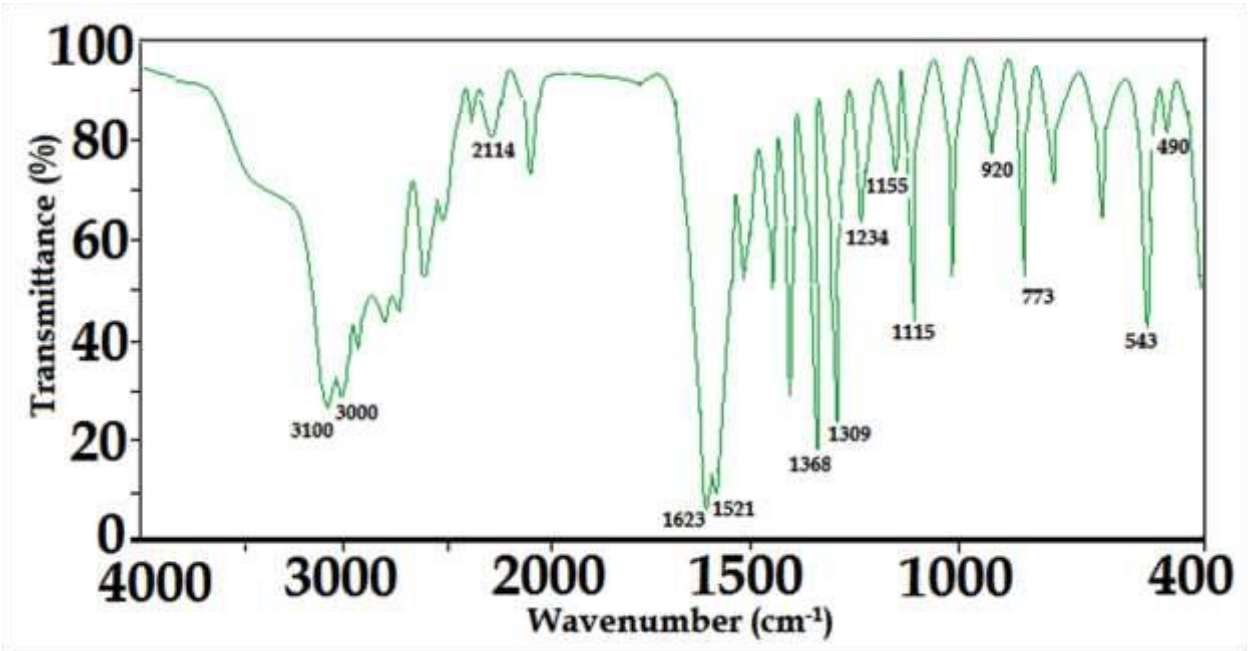

Fig.2. FTIR- spectrum of 2APA

3.3 Proton $_1$H-NMR analysis

The $_1$H- NMR spectrum of the compound 2APA (Fig.3) using a JEOL: GSX 500 instrument in deuterated water. NMR technique is used to detect the presence of particular nuclei in a compound for a given nuclear species. It is also an important tool for the identification of molecules and the examination of their electronic structure. From this spectrum the peak observed at 1.72 ppm is assigned methyl protons. The signal 4.8 ppm is due to NH_3 proton and methane proton CH attributed at 3.74 ppm.

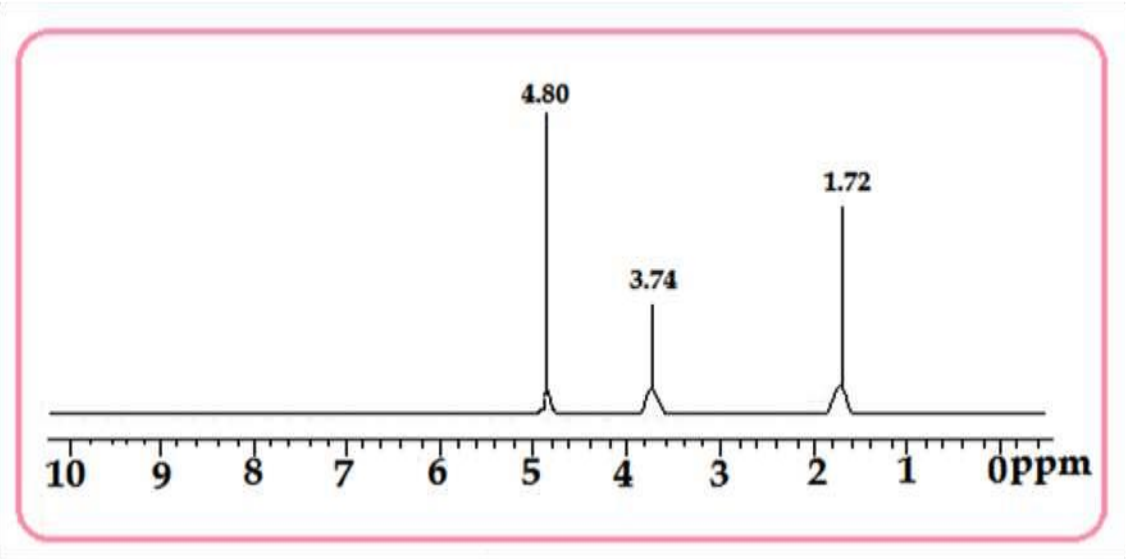

Fig. 3 Proton $_1$H-NMR spectrum of 2APA

3.4 UV-Vis-NIR spectroscopy

UV-Vis-NIR studies are carried out between 200nm-1000nm. The recorded absorption spectra of 2APA crystals are shown in figure 4. It shows that there no absorption in entire visible region. The absence of absorption of light in the visible region is an intrinsic property of all the amino acids. The maximum absorption lies around 242 nm. There is no absorption of light in the visible range of the electromagnetic spectrum, and it can be used as a potential material for SHG or other applications in the blue and violet regions.

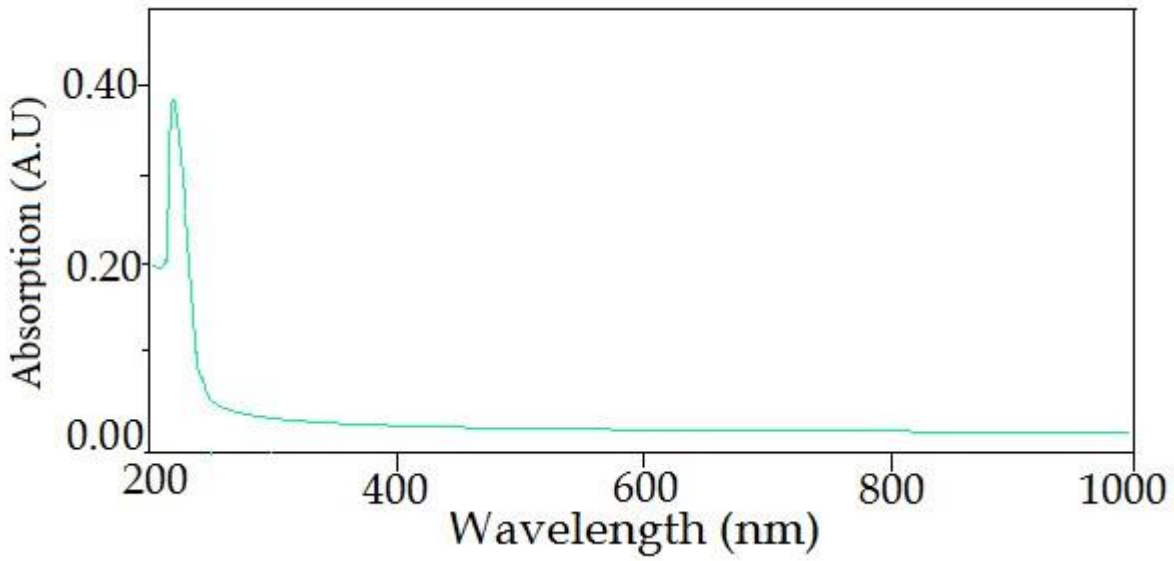

Fig. 4 UV-Vis-NIR spectrum of 2APA

3.5 Thermal analysis

Thermal analysis gives information about phase transition, water of crystallization and different stages of decomposition of the grown crystal [11].Thermo gravimetric (TG) and Differential thermal analysis (DTA) of 2APA shown in fig. 5 using perkin Elmer Diamond TGA-DTA equipment in nitrogen atmosphere at a heating rate of 10°C/min. for a range of 20 to 800°C to assess the thermal stability. From the TG curve it is understood that the 2APA is stable upto 296°C and decomposed immediately after melting. The DTA curve indicates the same changes shown by TGA curve. The sharp endothermic peak at 296 °C is the melting point of the 2APA.

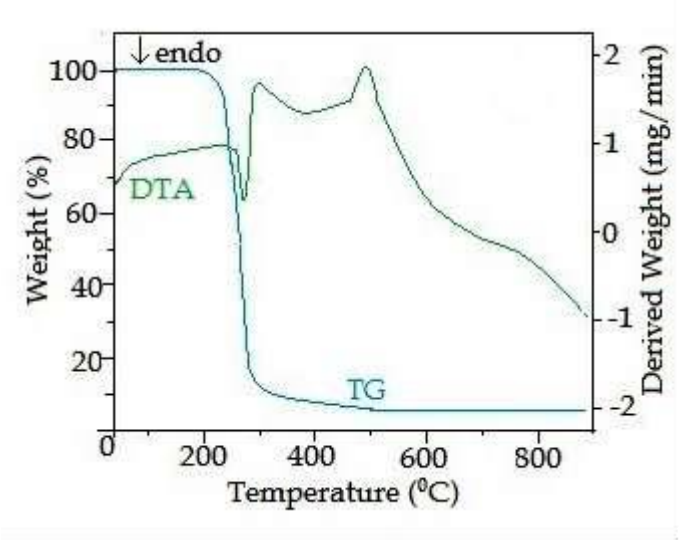

Fig. 5 TG-DTA spectrum of 2APA

3.6 NLO Test

Nonlinear optical (NLO) property of 2APA crystals was carried out from Kurtz powder test [12] using the Nd: YAG Q-switched laser beam. The grown crystals were ground to powder and packed between two transparent glass slides. The first harmonic output of 1064 nm from Nd:YAG laser was made to fall normally on the prepared crystal with pulse width of 8 ns, 10 Hz pulse rate and 6.2 mJ energy per pulse. The efficiency is confirmed with KDP and it is 0.3 times that of KDP.

IV. CONCLUSION

The single crystals of 2APA were successfully grown by the slow evaporation solution growth method. The grown crystal of 2APA has been subjected to various characterization studies. Single crystal XRD confirmed that 2APA belongs to orthorhombic system. The presence of various function groups in the title salt has been confirmed by FT-IR and proton $_1$H-NMR spectroscopic analysis. The minimum absorption in the visible region is observed from the UV-Vis measurement. It is a key requirement for the materials having NLO properties. The thermal analyses revel that the stability of the crystal was upto 296°C. The Second harmonic generation confirmed by Kurtz powder test.

REFERENCE

a) *[1] Suresh Sagadevan , Priya Murugasen, American Journal of Optics and Photonics, 2014; 2(5): 65-68*
b) *[2] Manoj, K.G., Nidhi, S.,and Binay, K., Physica B., 2011,406 (1), 63-67.*
c) *[3] T.F. Krauss and T. Baba, IEEE J. Quantum Electron.38 (2002) 724.*
d) *[4] R.M. Delarue, QuantumElectron. 34 (2002) 1.*
e) *[5] M.H.Jiang and Q.Fanng, Adv. Matter. 11 (1999) 1147.*

f) *[6] M.D.Aggarwal, J.Choi, W.S.Wang, K.Bhat, R.B. Lal, A.D. Shields, et al, J. Cryst Growth179,(2004).*

g) *[7] Lydia Caroline M., Sankar R., Indirani R.M and Vasudevan S. (2009), Materials Chemistry and Physics, Vol. 114, pp. 490-494.*

h) *[8] A. Wojciechowski, K. Ozga, A. H. Reshak et al., Materials Letters, vol. 64, no. 18, pp. 1957–1959, 2010.*
i) *[9] L. Misoguti, A.T.Varela, F.D.Nunes, V.S.Bagnato, F.E. Melo, J. Mendes Filho, S.C. Zilio, S. C. Opt. Mater.* ***1996****, 6, 147-152.*
j) *(10) C. Razzetti, M. Ardoino, L. Zanotti, M. Zha, C. Paorici, Cryst Res. Technol.* ***2002****, 37, 456-465.*

k) *[11] F.Q. Meng, M.K. Lu, Z.H. Yang, H. Zeng, Mater. Lett. 33(1998) 265–268*
l) *[12] S.K. Kurtz, T.T. Perry, J. App. Physics 39 (1968) 3798.*

International Journal of Research in Science advanced Technology and management studies (IJRSTMS)

ISSN: 2459-425X • Website: www.ijrstms.com