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GROWTH AND CHARACTERIZATION OF NONLINEAR OPTICAL MATERIAL: ALANINE BARIUM CHLORIDE

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ABSTRACT

Single crystals of Alanine Barium Chloride (ABC), a semi organic nonlinear optical material has been grown from solution by slow evaporation at ambient temperature. The growth of crystals has been carried out at various pH values and the growth was confirmed at pH 5.7. The chemical composition of the grown crystals was determined by the FTIR spectra. The crystalline nature and its various planes of reflections were observed by the powder XRD and single crystal XRD. The structure is built from alternate layers of L-alanine organic molecules and inorganic layers consisting of Ba^+ ions and Cl^- ions. The Hardness of the crystal was studied by Vickers micro hardness measurement. The transmittance and absorption of the crystal was studied by UV-Vis spectrometer.

Key words : 1.Characterization; 2.X-ray diffraction; 3. Growth from solutions; 4.Non-linear optic materials.

INTRODUCTION

In recent years, organo-inorganic hybrid materials have attracted considerable attention. In particular, the inorganic derivatives of protein amino acids are often attributed to symmetric groups without an inversion centre mostly to polar symmetry groups. Their crystals have properties whose symmetry is described by odd -rank tensors such as pyro-electric effect, spontaneous electric polarization, piezoelectric effect, generation of second optical harmonics, etc. Moreover crystals that belong to the eleven enantiomorphic point groups, having no mirror reflection planes exhibit optical activity, which is described in terms of the axial generation tensors [1-5]. While the structures of most amino acids are well defined, the structures of the derivatives of the protein amino acids with inorganic components are not. This paper defines the crystal structure of alanine barium **c**hloride [ABC]. This has been investigated by the FTIR studies, its crystalline nature is studied by the powder XRD, the transmittance and absorbance of electromagnetic radiation is studied through UV-Visible spectrum.

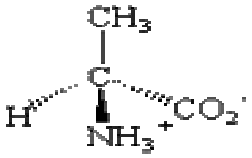
EXPERIMENTAL

Synthesis and crystal growth

A Solution was prepared using $BaCl_2.(2H_2O)$ and L-alanine in the molar ratio of 1:1. This solution was prepared using 25 ml of distal water and the super saturation was obtained after adding 12gms of L-alanine and $BaCl_2.(2H_2O)$ salt. The pH of the solution is adjusted to 5.7 by adding 2 to 3 drops of dilute hydrochloric acid. Seed crystals were obtained after one week. These seed crystal were used for the growth of bulk alanine barium chloride crystals[4].

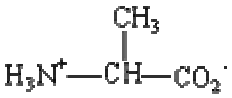
Structure of L-alanine molecule

The α-carbon atom of L-alanine is bound with a methyl group ($-CH_3$), making it one of the simplest α-amino acids with respect to molecular structure and also resulting in L-alanine being classified as an aliphatic amino acid. The methyl group of L-alanine is non-reactive and is thus almost never directly involved in protein function. The structure of L-alanine is-



L-alanine

Further its linear zwitter ionic structure is



The crystal structute of L-alanine is orthorombic. Its cell parameters are
A = 6.032, b= 12.343, c = 5.784 [1].

Characterization

X-RAY diffraction

The grown crystals have been characterized by powder X-ray diffractometer. Fig.-1 represents the powder X-ray pattern of the grown GSC. The lattice parameter values of glycine sodium chloride (GSC) taken from the literature were used for the simulation of hkl values and corresponding d values have been calculated. The single crystal X-ray diffraction analysis has been performed using the single crystal X-ray diffractometer on alanine barium chloride (ABC) crystals and the obtained crystallographic data are given in table1. The system is found to be Orthorhombic.

Powder XRD interpretation

The powder XRD for the grown crystal alanine barium chloride is taken the XRD curve source that the material alanine barium chloride is crystalline nature. The planes of reflection are shown in the graph that is the graph is indexed. The x-axis of graph is 2θ. The y-axis gives the intensity the units are arbitrary

Singel crystal XRD interpretation

A single crystal XRD revealed that the cell parameters of alanine barium chloride (ABC) as-

$a=5.797(7)\ A^0$
$b=6.050(7)\ A^0$
$c=12.387(14)\ A^0$

V(volume the crystal) $= 434\ A^{03}$

$\alpha = \beta = \gamma = 90^0$

The crystal system is orthorhombic.

FT-IR spectra

The FTIR spectrum of alanine barium chloride reveals the following fetch. 3417cm^{-1} with medium intensity refers to a primary amine free radical with N-H symmetric stretching mode of vibration. 2601cm^{-1} [2] with week band refers to overtones the formation of OH in-plane will be and C-O stretching vibration. From which we infer that band refers to carboxylic acid. 2249cm^{-1} with strong intensity band refers to NH_4 stretching which can be inferred as tertiary amine salt. 1413 cm^{-1} medium band refers to C-H in-plane-bending. 769cm^{-1} with[3] strong band refers to C-Cl stretching from which we infer crystal contain chloride radical.

UV-Visible spectra

The light of wavelength 193.4 nm is absorbed. This is the cut of point. Then the crystal is highly transparent to the wave lengths above 193.4nm up to 1200nm. From this UV spectrum we infer that crystal may have NLO property.

Micro hardness (Fig. 4)

The micro hardness number decreases with increasing in the load. So the brittleness of the crystal for the load is large. Even with the small increase in the load hardness number is large. So the crystal is soft.

RESULTS AND DISCUSSION

The seed crystals of alanine barium chloride (ABC) are grown from the solution prepared from the raw materials L-alanine and barium chloride of 99.99 percentage of purity. These crystals are characterized and the following results are obtained.

1. From the powder XRD pattern we infer that the material ABC is crystalline and the system is orthorhombic.
2. Further the FTIR spectrum reviles the structure of the alanine barium chloride (ABC).Moreover the crystal is also transparent to the Infrared rays.
3. From the UV-Visible spectrum of the martial ABC we find that this material is transparent to all the wavelengths of visible and UV. From this we can conclude that the crystal may have second order harmonic generation.
4. From the micro hardness study of the material ABC we find the material is soft.

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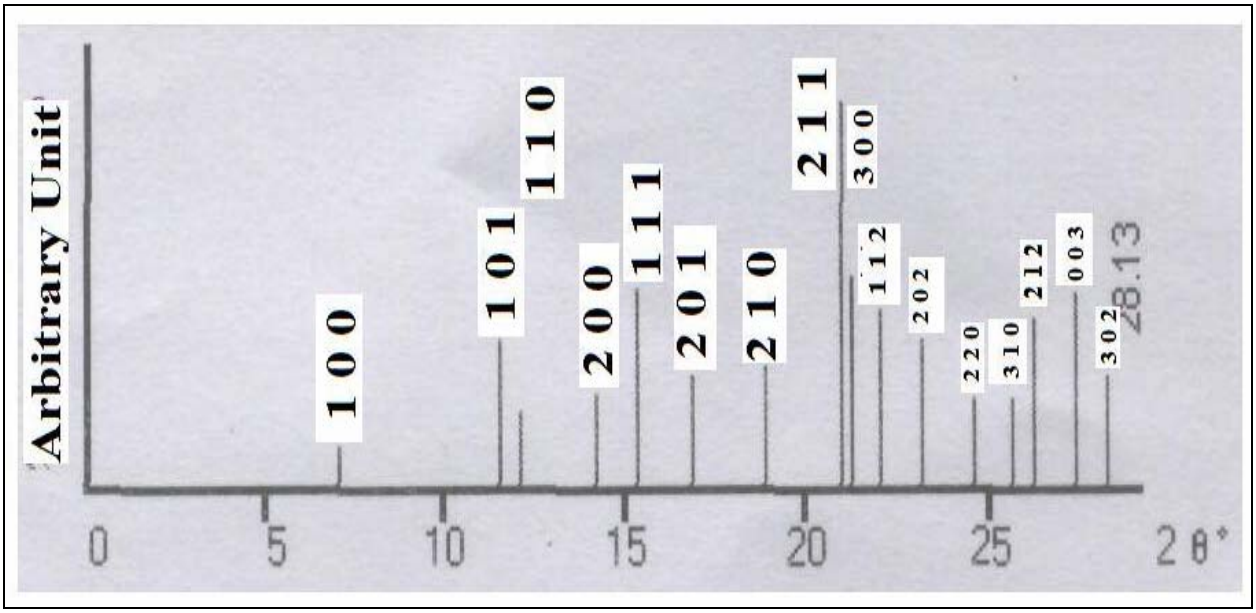
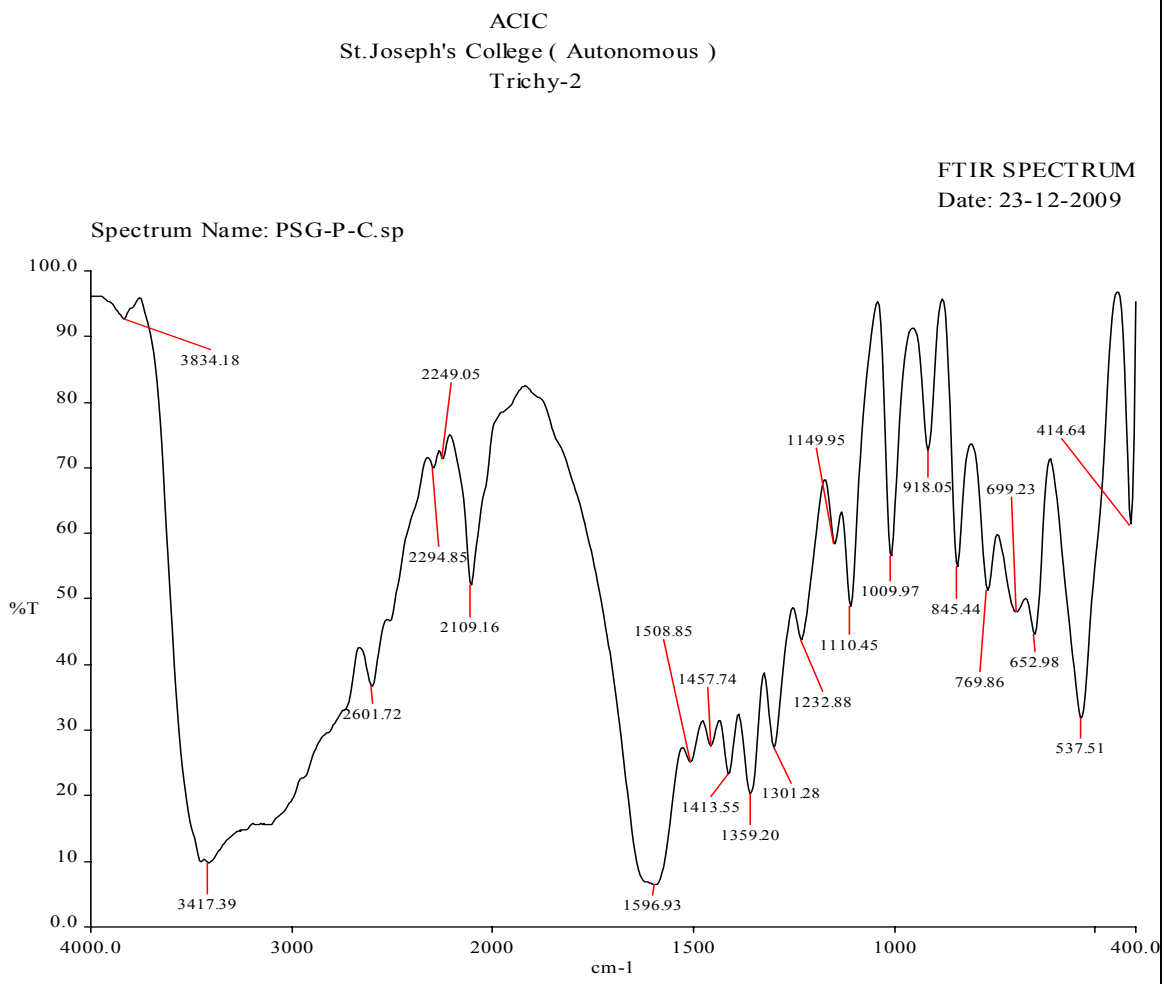


Fig.-1:Powder XRD Pattern of Alanine Barium Chloride (ABC).



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1009.97 56.63 918.05 72.58 845.44 54.94 769.86 51.26 699.23 48.01
652.98 44.61 537.51 31.82 414.64 61.34

Fig.-2: FTIR Spectrum of Alanine Barium Chloride (ABC).

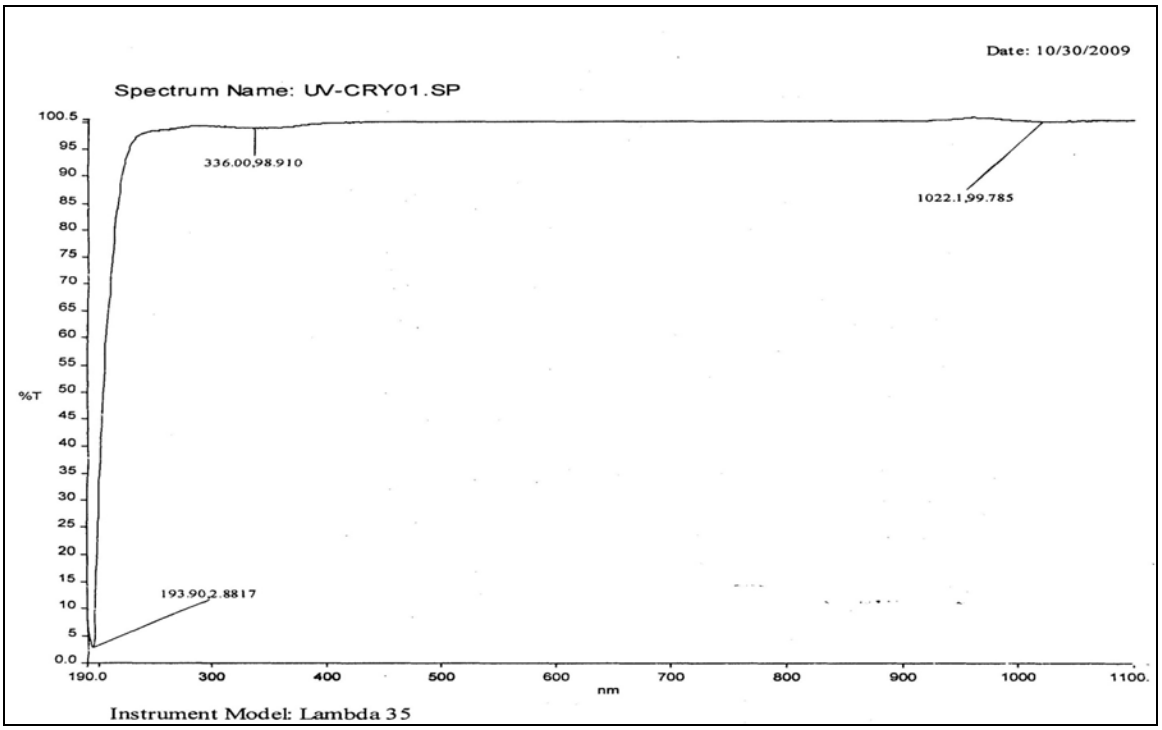

Fig.-3a: UV – Visible spectra of Alanine Barium Chloride (ABC) .

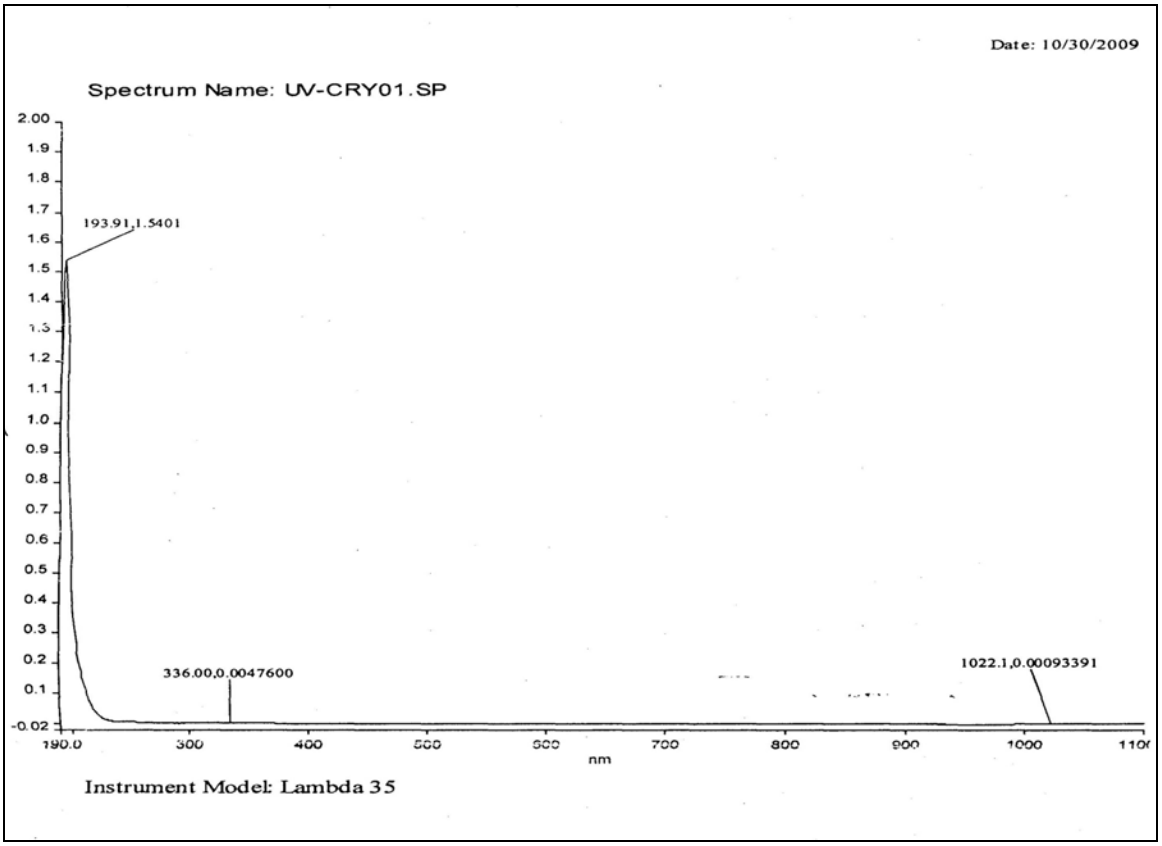

Fig.-3b: UV – Visible spectra of Alanine Barium Chloride (ABC).

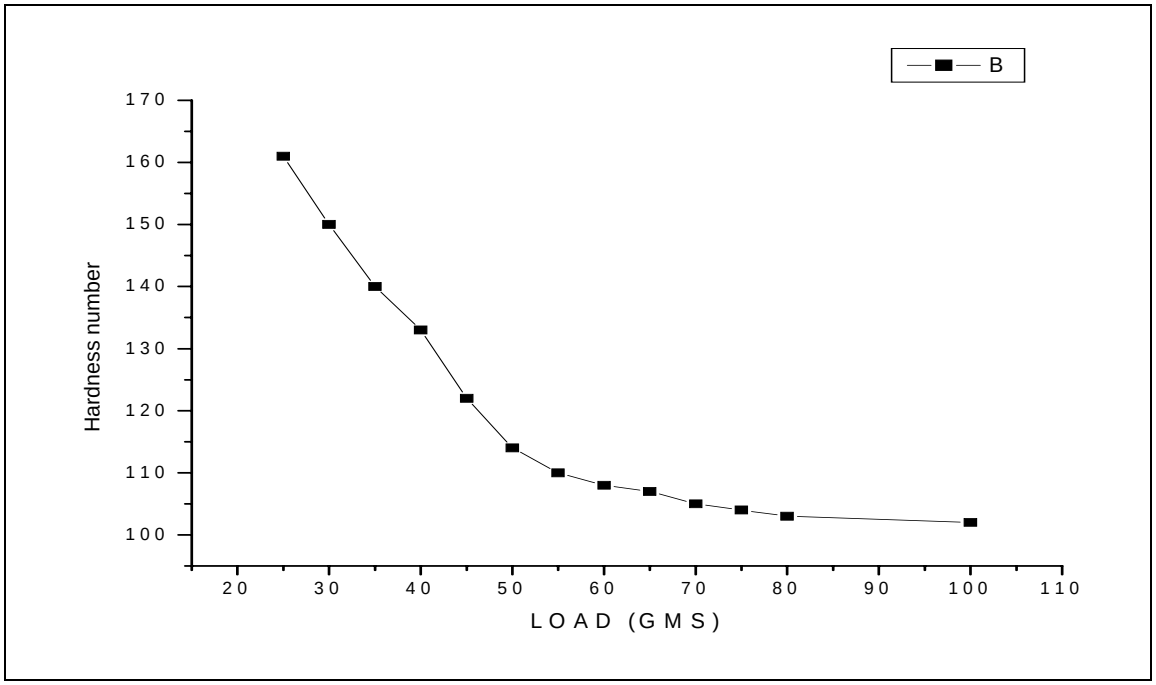

Fig.-4: variation of micro-hardness number with load.

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