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Optical And Electrical Properties Of L-Ornithine Hydrogen Bromide (L-Ohb) Single Crystal

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Abstract: ***L-Ornithine Hydrogen Bromide (L-OHB) crystal, one of the organic crystals, was grown by slow evaporation technique at room temperature. The as-grown crystal (L-OHB) is more transparent with dimensions 10× 5 × 3mm³. The incorporation of hydrogen bromide into the lattice site of L-Ornithine mono hydrochloride was confirmed using single crystal XRD. The fundamental functional groups of L-OHB were identified using FTIR spectral studies. The cut-off wavelength and band gap were determined from UV-vis-NIR absorption spectra and Tauc's plot respectively. The ac and dc electrical conductivities of the grown crystal were measured using LCR meter at various temperatures and the activation energy was calculated to analyse the electrical property of the material.***

Keywords: Slow evaporation, XRD, FTIR, UV-vis-NIR, electrical conductivity

1. Introduction

In recent years, the field of crystal growth has drawn much attention of the young researchers due to the rapid development in the optical modulation, optical switching and optical storage technology [1]. L-Ornithine Hydrogen Bromide (L-OHB) belongs to amino acid group which finds applications in optoelectronics and photonics. When it is combined with arginine, it also promotes bioactivity besides NLO activity. Amino acids are interesting organic materials with Zwitterionic nature having proton donor (COOH) and proton acceptor (NH_2) groups which have better probability of combining with other compounds [2-3]. In the present study, we report the growth and characterization of a novel organic crystal L-Ornithine Hydrogen bromide.

2. Experimental Procedure

Commercially available L-Ornithine mono hydrochloride and hydrogen bromide with 99.8% purity were taken in stoichiometric ratio 1:1 and dissolved in the double distilled water. The solution was stirred well for about 24 hrs to ensure homogeneity. The pH value of the solution was maintained at 3.5 which lies in the conducive range (3-4) for the growth of the crystal. The solution was allowed to evaporate gradually for achieving supersaturation. After a period of 25 days, needle shaped crystals were obtained. A well prominent transparent seed crystal was chosen and was grown in bulk form using hanging drop method. The photograph of the as-grown crystal with dimensions of 10× 5 × 3mm^3 is shown in Fig.1.

Figure 1: As-grown crystal L-OHB

3. Results and Discussion

3.1 Single Crystal XRD

The grown crystal was then subjected to single crystal XRD using ENRAF NONIUS CAD X-ray diffractrometer to determine the cell parameters. XRD data reveal that the grown crystal belongs to monoclinic system with space group $P2_1$. The lattice parameters are found to be a=5.01 Å, b=8.02 Å, c=10.10 Å; $\alpha = \gamma = 90^0$, $\beta = 97.46^0$ and V=410 $Å^3$.

3.2 Ftir Analysis:

FTIR spectrum (Fig.2) of L-OHB was recorded using PerkinElmer spectrometer in the range 0 -4500cm^{-1}. The presence of COO^- rocking and COO^- scissoring were observed at 459cm^{-1} and 667 cm^{-1} respectively. The characteristic bands of NH_3 torsion, NH_3 rocking and NH_3 symmetric deformation were identified at 553 cm^{-1}, 1138 cm^{-1} and 1625 cm^{-1} respectively. A broad band at 3099 cm^{-1} represents NH_3^+ symmetric stretching. The presence of NH_3

and COO^- confirms the amino acid group [4]. The frequency assignments of FTIR spectrum is shown in **Table 1**.

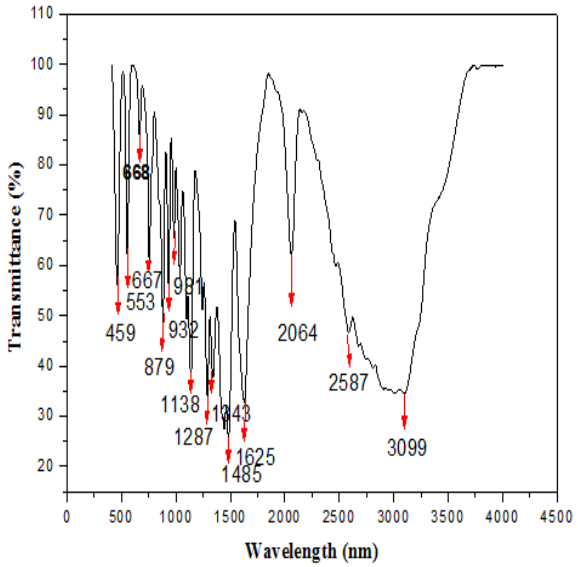

Figure 2: FTIR spectrum of L-OHB

Table 1: FTIR frequency assignment of L-OHB

Wave numbers (cm^{-1})	Frequency assignment
459	COO^- rocking
553	NH_3 torsion
667 &668	COO^- scissoring
932 & 981	C-C skeletal stretching
1138	C-C-N asymmetric stretching
1287 & 1485	CH_2 twisting
1342	NO_3 asymmetric stretching
1625	NH_3 symmetric deformation
2064 & 2587	Overtones and combination bands
3099	NH_3^+ symmetric stretching

3.3 Uv-Vis-Nir Spectrum Analysis

Fig.3 shows the UV-vis-NIR spectrum recorded in the range 200-1100nm. The material shows a transparent nature from 239nm onwards. The lower cut-off wavelength of the as-grown crystal was found to be 212nm. The optical band gap of L-OHB was estimated using Tauc's relation [4] given by

$$\alpha = \frac{(h\nu - E_g)^{1/2}}{h\nu} \quad (1)$$

where α is the absorption coefficient, E_g is optical band gap and hν is the photon energy (eV). The band gap was calculated from the plot of $(\alpha h\nu)^2$ versus hν as shown in Fig.4 The calculated band gap of L-OHB crystal was found to be 5.5eV. From the larger value of band gap, it is concluded that the material is dielectric in nature suitable for induced polarization.

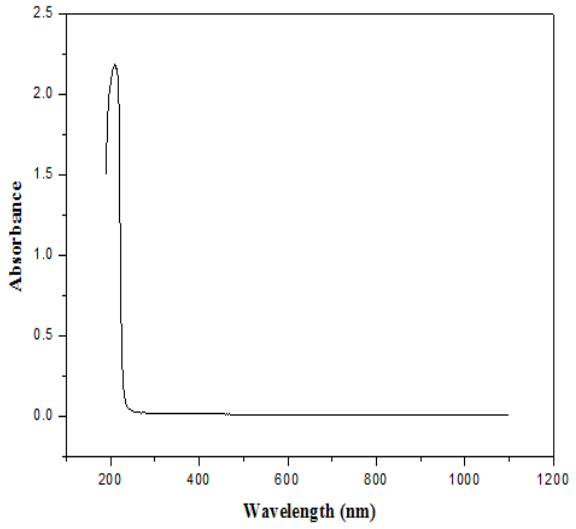

Figure 3: Optical absorption spectrum of L-OHB

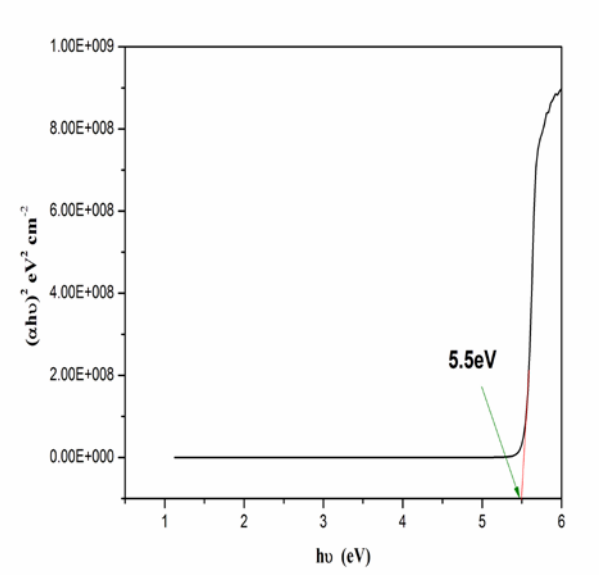

Figure 4: Optical bandgap of L-OHB

3.4 Electrical Conductivity

The ac conductivity and dc conductivity of the grown crystal were measured using LCR meter at different frequencies and temperatures. The ac and dc conductivity were calculated using the formulae[5-6],

$$\sigma_{ac} = 2\pi f \varepsilon_0 \varepsilon_r \tan\delta \quad (2)$$

and

$$\sigma_{dc} = d/RA \quad (3)$$

where f is the frequency, ε_0 is the permittivity of free space, ε_r is the relative permittivity of the medium and T is the temperature; d is the thickness, R is the resistance and A is the area of cross-section of the material.

The electrical conduction in the sample is a thermally activated transport process which is governed by the following Arrhenius type of equation,

$$\sigma = \sigma_0 \exp(^{-E_a}/_{kT}) \qquad (4)$$

where E_a is the activation energy, k is the Boltzmann constant and T is the temperature.

Fig. 4(a) shows the plot of $\ln\sigma_{ac}$ versus 1000/T at different frequencies. It is understood that ac conductivity increases with increase in temperature and frequency. The activation energy for ac conductivity was calculated from the slope of the plot as 0.18eV.

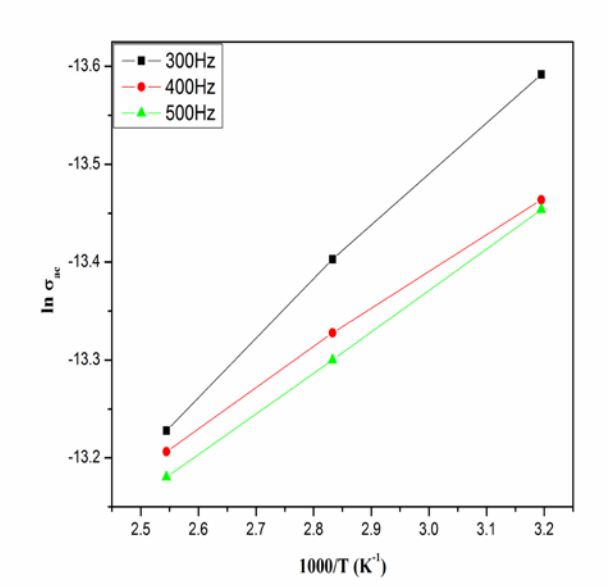

Figure 4 (a): AC conductivity as a function of temperature at different frequencies

Fig.4(b) shows the plot of ln σ_{dc} versus 1000/T. It is observed that the dc conductivity also increases with temperature. The activation energy for dc conductivity was calculated as 0.3eV. The lower values of activation energy for both ac and dc electrical conductivities suggest that the grown material has minimum density of defects.

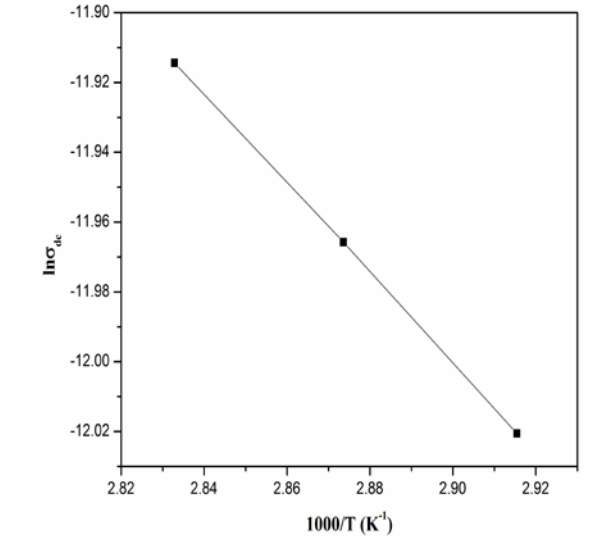

Figure 4 (b):DC conductivity as a function of temperature

4. Conclusion

L-OHB was grown using slow evaporation technique. The monoclinic crystalline nature was confirmed by single crystal XRD. The functional groups such as COOH, NH_3, CH_2 etc., have been identified from FTIR spectrum. The activation energies were calculated as 0.18eV and 0.3eV for both ac and dc conductivities.

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