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Short Communication

Investigations on Growth, Theoretical and Dielectric Properties of L-Glutamic Acid Hydrobromide (GHB) NLO Single Crystal

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Abstract

Single crystals of L-glutamic acid hydrobromide (GHB) were grown from aqueous solution by slow evaporation technique. Single crystal X-ray diffraction analysis shows that the crystal belongs to monoclinic system with the space group $P2_12_12_1$. Several solid-state physical parameters have been determined for the grown single crystals. The dielectric constant and the dielectric loss of the grown crystal were studied as a function of frequency at room temperature.

Keywords: Single crystal, growth from solution, X-ray diffraction, dielectric constant and dielectric loss.

Introduction

The nonlinear optical properties of the organic molecular crystals have received a great deal of interest for the past two decades due to their extensive application in the fields like laser technology, telecommunication, optical information processing and storage[1,2]. The nonlinear response of the crystal is due to the application of strong sources of electric field which gives rise to the second and higher order nonlinear properties like second harmonic generation, d-c rectification, three frequency generation such as mixing, sum generation, self focusing, Kerr effect[3], two photon absorption and Raman scattering. One can explore all these nonlinear effects from the asymmetric systems by attributing them into high intense optical beam. The linear properties of all the centrosymmetric systems could be given by second rank tensor $\chi^{(1)}$. In general, the effect of second harmonic generation (SHG) described by the third rank polar tensor $\chi^{(2)}$ is forbidden in linear systems but it is predominant in non-centrosymmetric systems. The performance of the organic NLO materials in the optical region placed a great demand on these materials owing to which, several attempts have been made by the scientists to identify the good quality nonlinear organic crystals. In this work an attempt has been made to locate a new class of organic NLO materials involving charge transfer from donor to acceptor followed by proton transfer from the acceptor. This paves the way for the formation of intermolecular hydrogen bonding, which is the root cause for the NLO property in such materials[4]. In the present study, growth has been carried out by using slow evaporation technique[5] and some solid–state physical parameters such as valance electron plasma energy, Penn gap, Fermi energy and electronic polarisability have been determined for L-glutamic acid hydrobromide single crystal. The dielectric constant and the dielectric loss have been determined as a function of frequency at room temperature for the L-glutamic acid hydrobromide single crystal.

Material and Methods

Crystal growth: Single crystal of GHB were grown from L-Glutamic acid and hydrobromic acid taken in the equimolar ratio in aqueous solution by slow evaporation method. The solution was stirred continuously using magnetic stirrer for 3 days. The prepared solution was filtered and kept undisturbed at room temperature. Tiny seed crystals with good transparency were obtained due to the spontaneous nucleation. Among them, defect free seed crystal was suspended in the mother solution, which was allowed to evaporate at room temperature. Large size single crystals were obtained due to collection of monomers at the seed crystal sites from the mother solution. Figure 1 shows as grown single crystal of GHB.

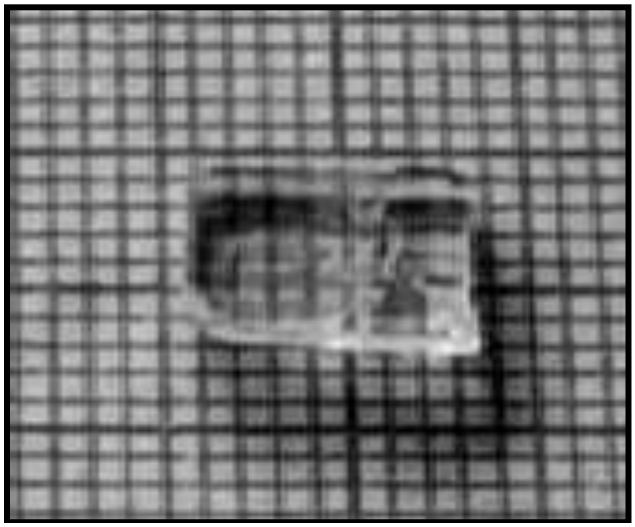

Figure 1
Photograph of a GHB crystal

Results and Discussion

Single-crystal X-ray diffraction and fundamental parameters: From the single crystal X-ray diffraction data, it was confirmed that the grown crystal belongs to orthorhombic system with the non-centrosymmetric space group of $P2_12_12_1$. The cell parameters are: a = 5.37 Å, b = 11.75 Å, c = 13.39 Å. These values agreed well with the reported values [5]. The molecular weight of the grown crystal is *M*=221 g, and total number of valence electron *Z*=54**.** The density of the grown crystal was found to be ρ=1.42 g cm^{-3} and dielectric constant at 1 MHz is ε_∞ =187.6. The valence electron plasma energy, $\hbar\omega_P$ is given by

$$\hbar\omega_P = 28.8\left(\frac{Z\rho}{M}\right)^{\frac{1}{2}} \quad (1)$$

where Z is the total number of valence electrons, ρ is the density and M is the molecular weight of the GHB single crystal. The Plasma energy is terms of Penn gap and Fermi energy [6] in eV is given as

$$E_p = \frac{\hbar\omega_P}{(\varepsilon_\infty - 1)^{1/2}} \quad (2)$$

and

$$E_F = 0.2948(\hbar\omega_P)^{4/3} \quad (3)$$

Polarizability, α is obtained using the relation [7]

$$\alpha = \left[\frac{(\hbar\omega_P)^2 S_0}{(\hbar\omega_P)^2 S_0 + E_g C}\right] \times \frac{M}{\rho N_a} \quad (4)$$

where S_0 is a constant for a particular material and is given by

$$S_0 = 1 - \left[\frac{E_P}{4E_F}\right] + \frac{1}{3}\left[\frac{E_P}{4E_F}\right]^2 \quad (5)$$

The value of α so obtained agrees well with that of Clausius-Mossotti equation, which is given by,

$$\alpha = \frac{3M}{4\pi N\rho}\left(\frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 2}\right) \quad (6)$$

where the symbols have their usual significance. N_a is Avagadro number and the calculated fundamental data on the grown crystal of GHB are listed in table1.

Table-1
Some theoretical data for GHB single crystal

Parameters	Values
Plasma energy (eV)	22.46
Penn gab (eV)	2.11
Fermi gap (eV)	18.24
Polarizability (cm^3) Penn analysis	7.203 x 10^{-23}
Polarizability (cm^3) Clausius-Mossotti Equation	7.121 x 10^{-23}

Dielectric studies: Single crystal of GHB was subjected to dielectric studies using a HIOKI HITESTER MODEL 3532-50 LCR meter and conventional two terminal sample holder. Dielectric permittivity measurements were carried out with the sample of dimension 2 × 2 × 1 mm^3 have been placed inside a dielectric cell whose capacitance were measured at room temperature for different frequencies. The techniques used for the measurement of dielectric constant are either reflection coefficients or resonant frequencies. In the later case, material is characterized to load a resonant cavity and the sample permittivity is evaluated from the shift of the resonant frequency value compared to that of the empty (unload) cavity. The dielectric constant and dielectric loss have been calculated using the equations (7) and (8).

$$\varepsilon = \frac{Cd}{A\varepsilon_0} \quad (7)$$

$$\varepsilon' = \tan\delta \quad (8)$$

Where d is the thickness of the sample, A is the area of the sample. The observations are made in the frequency range 50 Hz to 5 MHz at room temperature. Figure 2 and 3 represent the plots of dielectric constant and dielectric loss against frequency. From the graph it is observed that dielectric constant is maximum at 100 Hz since all types of polarization such as electronic, ionic, orientation and space charge polarizations occur at lower frequency. Figure 3, it is observed that the dielectric loss decreases with increase in frequencies at room temperature. Because of the inertia of the molecules and ions at high frequencies, the orientation and ionic contributions of polarization are small[8]. So, the magnitude of polarization increases with the decrease of frequencies.

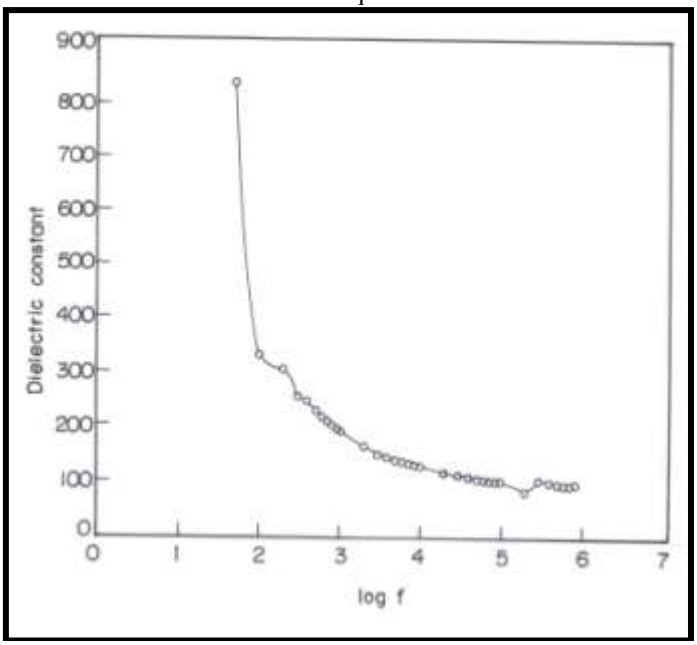

Figure-3
Dielectric constant vs log f

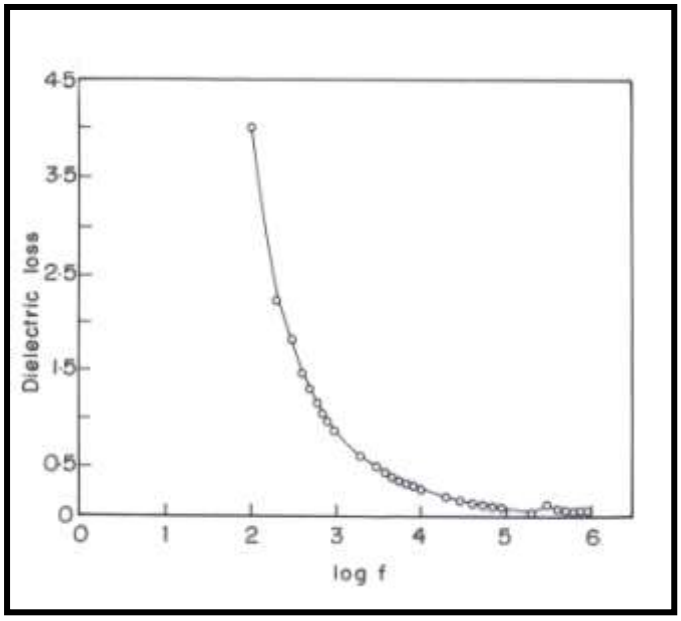

Figure-4
Dielectric loss vs log f

Conclusion

Single crystals of GHB were grown by using the slow evaporation technique. The lattice parameters were calculated by single crystal X-ray diffraction and it was confirmed that the crystals belong to the monoclinic system with the space group $P2_12_12_1$. The physical parameters such as valence electron plasma energy, Penn gap, Fermi energy and electronic polarisability have been determined for the GHB crystal. The variation of dielectric constant and dielectric loss were studied as a function of frequency at room temperature.

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