

Studies on Optical, Dielectric and Electrical Conductivity Properties of Zinc Succinate NLO Single Crystal

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ABSTRACT

Single crystals of Zinc Succinate (ZS) have been successfully grown from aqueous solution by slow evaporation method. Single crystal X-ray diffraction analysis reveals that the crystal belongs to monoclinic system with the space group C2. The optical transmission study reveals the transparency of the crystal in the entire visible region and the cut off wavelength has been found to be 320 nm. The optical band gap is found to be 3.60 eV. Dielectric constant and dielectric loss measurements were carried out at different temperatures and frequencies. AC electrical conductivity and photoconductivity studies are also carried out and the results are discussed.

Key words: Solution growth, Single crystal XRD, Optical transmission, Dielectric studies, Photoconductivity.

INTRODUCTION

Nonlinear optics (NLO) deals with the interaction of applied electromagnetic fields in various materials to generate new electromagnetic fields, altered in frequency, phase, or other physical properties. NLO is one of the few modern scientific frontiers where the interest is not only for understanding of new physical phenomena, but also to realize the technological applications. Nonlinear optical (NLO) materials are used in optical computing, optical communication, harmonic generators, medical diagnostics, frequency mixing and optical switching [1] and [2]. The potential development of optoelectronic devices based on the nonlinear polarization of molecular materials has aroused much recent interest [3] and [4]. Nonlinear optical materials have gained importance due to their pertinent properties such as high laser damage threshold, wide transparency range and high nonlinear coefficient [5-6]. These applications depend upon the various properties of the materials, such as transparency, birefringence, laser damage threshold, hardness, dielectric constant, thermal, photochemical and chemical stability. In the present investigation, deals with the growth of zinc succinate single crystal by the slow evaporation technique. The grown crystal has been subjected to single crystal XRD, Optical transmission, dielectric, AC electrical conductivity and photoconductivity studies.

MATERIALS AND METHODS

Single crystals of the title compound zinc succinate were grown by slow evaporation technique at room temperature. The growth solution of the title compound was prepared by taking equimolar ratio of hexahydrate zinc nitrate and succinic acid in aqueous solution. Deionised water was used as solvent and on repeated recrystallization; bright and optically transparent single crystals were harvested in about four weeks. 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.

RESULTS AND DISCUSSION

3.1 Single-crystal X-ray diffraction

Single crystal data collection was performed by using ENRAF NONIUS CAD-4 X-ray diffractometer. The XRD study reveals that the crystal belongs to monoclinic system with lattice parameters $a = 7.52 \text{ \AA}$, $b = 5.93 \text{ \AA}$ and $c = 6.22 \text{ \AA}$, and space group is $C2$, which is in agreement with reported values [7].

3.2 Optical Transmission Studies

The optical transmission spectrum was recorded in the range of 190–1700 nm. The spectrum is shown in Figure.1. From the transmission spectrum it is observed that the crystal has good transmission in the entire visible and IR region and the lower cutoff of the ZS is at 330 nm. The absence of absorption in the region between 320 and 1150 nm shows that this crystal could be used for optical window applications.

The measured transmittance (T) was used to calculate the absorption coefficient (α) using the formula

$$\alpha = \frac{2.3026 \log\left(\frac{1}{T}\right)}{t} \quad (1)$$

where ' t ' is the thickness of the sample. Optical band gap (E_g) was evaluated from the transmission spectra and optical absorption coefficient (α) near the absorption edge is given by [8]

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

where A is a constant, E_g the optical band gap, h the Planck constant and ν the frequency of the incident photons. The band gap of ZS crystal was estimated by plotting $(\alpha h\nu)^2$ versus $h\nu$ as shown in Figure. 2. From the figure, the value of band gap was found to be 3.60 eV.

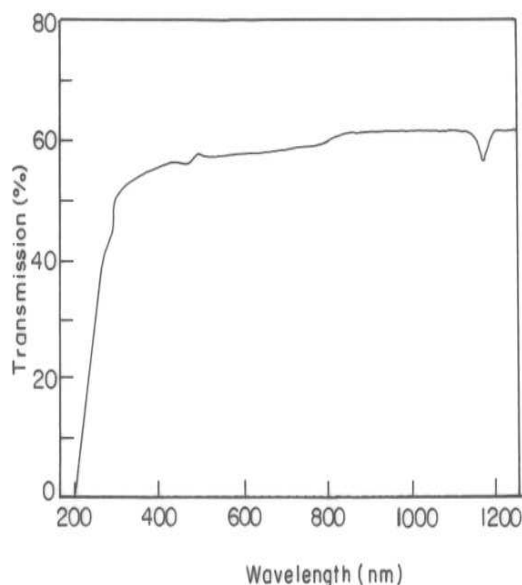


Fig.1. Optical transmittance spectrum

3.3 Dielectric studies

The dielectric constant and the dielectric loss of the ZS crystals were studied at different temperatures using HIOKI 3532 LCR HITESTER in the frequency region 50 Hz to 5 MHz. The dielectric constant was measured as a function of frequency at different temperatures ranging from 40 to 90°C and is shown in Figure.3, while the corresponding dielectric losses are depicted in Figure.4. It is observed from the plot (Figure.3) that the dielectric constant decreases exponentially with increasing frequency and then attains almost a constant value in the high frequency region. It is also observed that as the temperature increases, the value of the dielectric constant also increases. The same trend is observed in the case of dielectric loss versus frequency. The characteristic of low dielectric constant and dielectric loss with high frequency for a given sample suggests that the sample possesses enhanced optical quality with lesser

defects and this parameter is highly important for making this material suitable for various nonlinear optical applications.

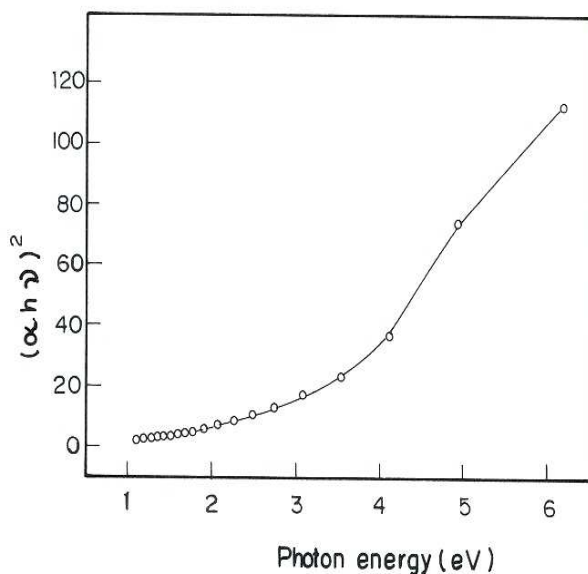


Fig. 2. $(\alpha h\nu)^2$ Versus $h\nu$

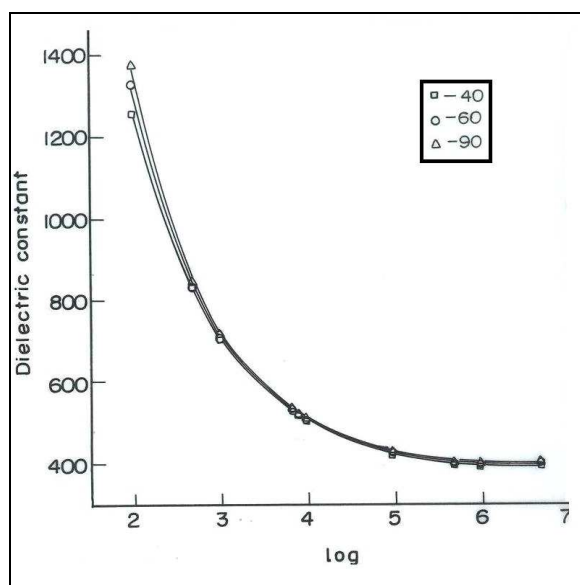


Figure 3. Dielectric constant vs log f

3.4 Electrical AC conductivity studies

The AC conductivity study of the ZS crystal was carried out at 1 KHz. In the high temperature (Intrinsic) region, the effect of impurity on electrical conduction has not made any appreciable change whereas in the low temperature (extrinsic) region, the presence of impurities in the crystal has an impact and particularly increases its conductivity.

The electrical conduction in dielectrics is mainly a defect controlled process in the low temperature region (Figure.5). The presence of impurities and vacancies predominantly affect the conductivity in this region. The energy needed to form the defect is much larger than the energy need for its drift. It is found from the Arrhenius plot (Figure.6) for the ZS crystal that the conductivity increases with temperature and the value of activation energy is found to be 0.110 eV. The conduction mechanism can be explained by the rotation of ions when the temperature of the material is increased. The rotation of ions gives local displacement of electrons in the direction of the applied field, which in turn gives rise to induced polarization when the material is subject to intense laser beam. The lower

value of activation energy (0.110eV) predicted in the present investigation suggests that the crystal is free from defects. When the crystal is free from defects, the hydrogen bond interactions will not be weakened.

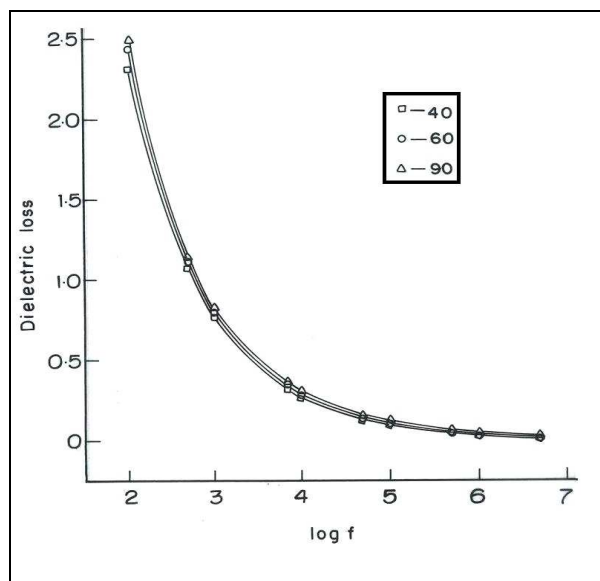


Figure 4. Dielectric loss vs log f

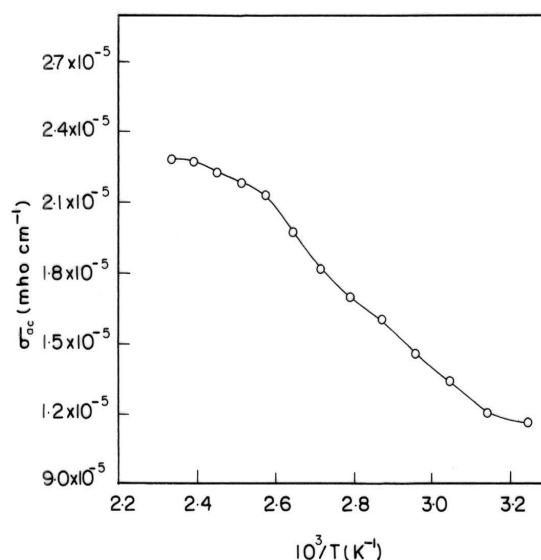


Fig. 5. Variation of ac conductivity with $1000/T$

3.5 Photoconductivity study

Photoconductivity measurements were made using Keithley 485 picoammeter. The dark current was recorded by keeping the sample unexposed to any radiation. Figure.7.shows the variation of both dark current (I_d) and photocurrent (I_p) with applied field. It is seen from the plots that both I_d and I_p of the sample increase linearly with applied field. It is observed from the plot that the dark current is always higher than the photocurrent, thus confirming the negative photoconductivity.

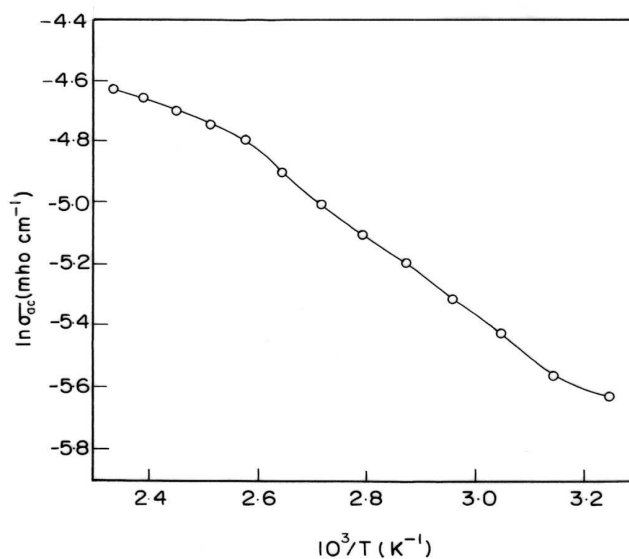


Fig. 6. Plot of $\ln(\sigma_{ac})$ vs $1000/T$

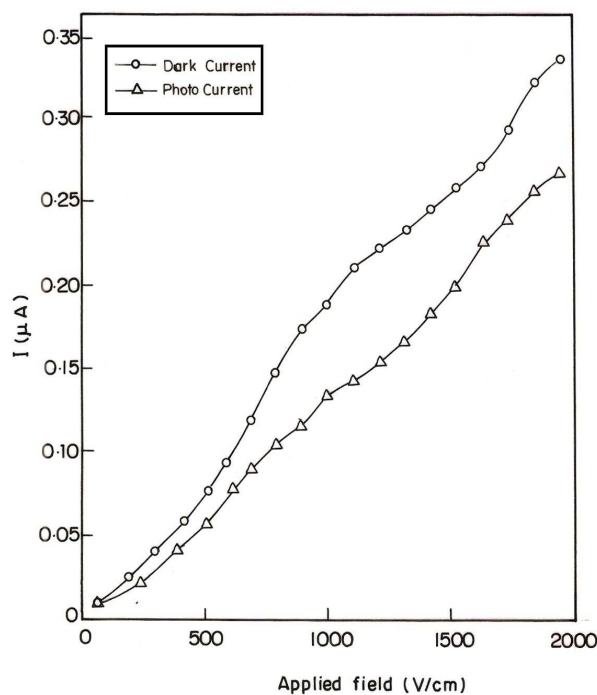


Fig.7. Field dependent photoconductivity of grown single crystal

CONCLUSION

Bulk single crystals of zinc succinate have been successfully grown by evaporation from aqueous solution. Single-crystal XRD analysis confirmed that the crystals belong to monoclinic system with the space group C2. The band gap energy of ZS estimated from the optical transmittance spectrum is about 3.60 eV. The dielectric constant decreases with increasing frequency at different temperatures. The activation energy was determined from the plots of ac conductivity. The photocurrent was less than the dark current, signifying negative photoconducting nature.

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