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Synthesis and Characterization of L-Proline Cadmium Chloride Monohydrate Single Crystal

J.P.Angelena*, M.Akilan, R.Ragu, J.Mary Linet, S.Jerome Das

Department of Physics, Loyola College, Chennai-600 034, India.

*Corresponding author: e-mail: angelenaj_81@yahoo.com

Abstract: ***The powder X-ray diffraction studies confirm the crystalline perfection of the grown L-PCCM single crystal. The grown crystal was characterized by single crystal XRD and confirmed that the crystal belongs to orthorhombic crystal system with lattice parameter P. The optical absorption study shows that L-PCCM was optically transparent in the entire visible and near IR region with a lower cut-off wavelength that 230 nm. The FT-IR spectrum reveals the mode of vibrations of different molecular groups present in the title compound. The characteristics of low dielectric loss for the sample suggest that it possesses enhanced optical quality with lesser defects and this parameter is of vital significance for nonlinear optical applications.***

Keywords: about four key words separated by commas**.**

1. Introduction

In the recent decade, it is essential to discover new materials with high NLO efficiency for application such as telecommunication, optical information processing, laser technology and other signal processing devices. Enormous developments have taken place in discovering new NLO materials having large nonlinear optical coefficients. The important factor for the selection of the material depends on the physical properties of the crystal and the prospects of the various applications [1-5]. Amino acids are important and interesting material for NLO application. Semi organic materials share the properties of organic and inorganic materials. A Polarizable organic molecule is stochiometrically bonded to an inorganic host to form compound of highly efficient optical quality organic based NLO crystals [6]. Organic NLO materials have good nonlinear optical coefficients but the mechanical and thermal properties are very low. The inorganic materials have excellent thermal and mechanical properties but low optical non linearity. To overcome these problems new types of hybrid NLO material have been explored from organic and inorganic complexes called semiorganic material. In the present study the single crystals of L-Proline cadmium chloride monohydrate (L-PCCM) a semi organic NLO compound has been synthesized and subjected to various characterization techniques.

2. Experimental Procedure

L-PCCM crystals were grown from an aqueous solution using the slow evaporation technique. L-Proline has two groups (an amino and guanadyl) which can be protonated. The material was synthesized by taking L-Proline and cadmium chloride in the stoichiometric ratio 1:1.The calculated amount of cadmium chloride was first dissolved in double distilled water. Then L-Proline was added to the solution slowly by stirring continuously for 2 hours to ensure homogenous concentration over the entire volume of the solution. The prepared solution was allowed to dry at room temperature to undergo slow evaporation. Well defined single crystals of good transparency were collected and it was shown in figure.2.1.

Figure 2.1: Photograph of Pure L-PCCM crystals

3. Results and Discussion

3.1 Single Crystal XRD

The grown crystals were subjected to single crystal X-ray diffraction using ENRAF NONIUS CAD-4 single-crystal X-ray diffractometer with MoKα radiation (λ = 0.7170 Å) to determine the unit cell dimensions. The pure crystal is found to be crystallized in the orthorhombic system with lattice parameter P. These values agree well with the reported values. The cell parameters of the grown crystal were listed in table 4.1.

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Table 3.1: Unit cell parameters of L-PCCM

Lattice parameters of L-PCCM	Crystal data
System	Orthorhombic
a	7.26 Å
b	9.95Å
c	13.48 Å
α	90^0
β	90^0
γ	90^0
Cell volume(V)	974 $Å^3$

3.2 Uv-Visible Spectral Studies

To explore the transmission range of L-PCCM for optical application, the UV-VIS transmittance spectrum was recorded with DRS-UV-VIS-NIR in the wavelength range of 200-800 nm using varian cary 5E UV-VIS-NIR Spectrometer. The crystal was found to be transparent and it is in good agreement with the reported values [9]. The main requirement for the materials having NLO properties is the absence of absorption. The UV absorption spectrum is plotted with the wavelength along X-axis and absorbance along Y-axis for a L-PCCM is shown in Fig 3.1. The maximum absorbance is at 200 nm. The UV cut off wavelength for L-PCCM is 230 nm.The crystal is transparent in the entire visible and near IR region. There is no absorption of light to any appreciable extent in the visible region of the electromagnetic spectrum which is an intensive property for device fabrication.

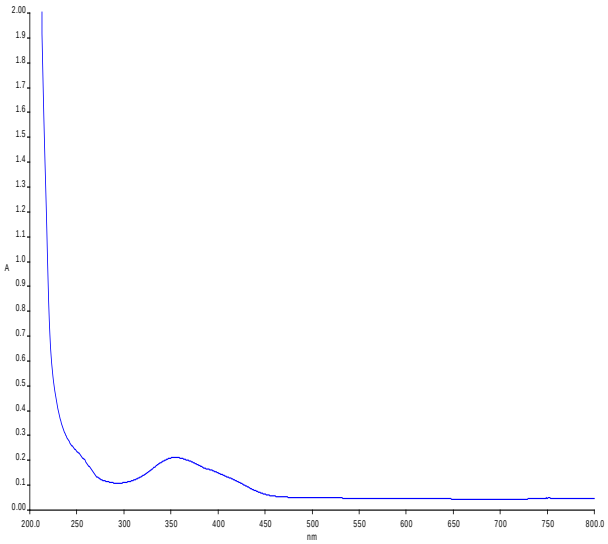

Figure 3.2. UV spectrum of L-PCCM crystal

3.3. FTIR Spectral Analysis

The FTIR analysis of the grown L-PCCM crystal was recorded in the frequency range 450-4000 cm^{-1} by using PERKIN ELMER SPECTROMETER. The FTIR spectral analysis of L-PCCM crystals is shown in Fig 3.2. In L-PCCM the peak at 3480 cm^{-1} is assigned to OH stretching vibration of H_2O (ii) CH_2 antisymmetric stretching mode is observed at 2990 cm^{-1} (iii) COO^- symmetric stretching is observed at 1433.(iv) wagging mode of NH_2 and CH_2 is observed at 1368 cm^{-1} and 1332 cm^{-1} (v) rocking mode of CH_2 and NH_2^+ is observed at 941 cm^{-1} and 916 cm^{-1} respectively.

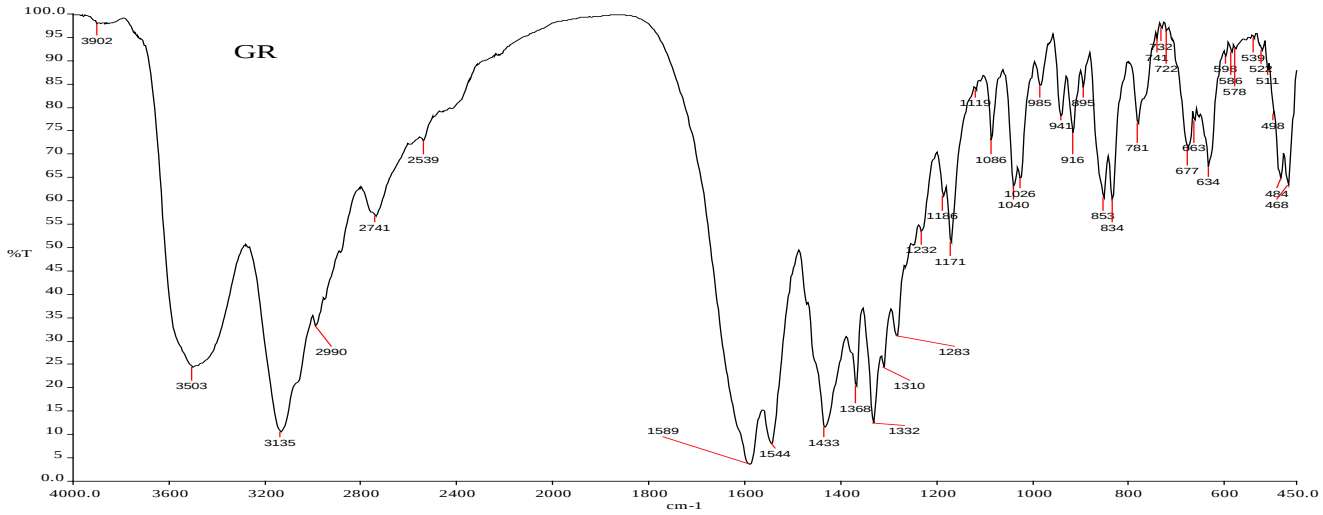

Figure 3.3. FTIR spectrum of L-PCCM crystal

Table 4.1: Vibrations of different functional groups of L-PCCM

Wave number cm^{-1}	Functional Groups
3902	OH stretching vibration of H_2O
3503	stretching Vibration of H_2O molecule.
2990	ν_a (Ch_2) antisymmetric stretching mode
1544	NH_2^+ in Plane deformation
1433	COO^- symmetric stretching
1368	wagging NH_2^+
1332	wagging CH_2^+
1171	wagging NH_2^+
1040	C-N stretch
941	rocking CH_2
916	rocking NH_2^+
853	rocking CH_2
781	n-plane deformation g COO^-
634	wagging COO^-
468	rocking COO^-

3.3 Dielectric Studies

The temperature dependent dielectric constant and loss of L-PCCM were measured using HIOKI 3532 LCR HITESTER in the frequency range of 100 Hz- 5 MHz in the temperature range of [RT-65]. It is seen from the Fig 3.3 & Fig 3.4 that both the dielectric constant and dielectric loss are inversely proportional to the frequency. The increase in dielectric constant at low frequency is due to space charge polarization. These curves suggest that the dielectric loss strongly depends on the frequency of the applied field similar to that of the dielectric constant which is common in ionic system.

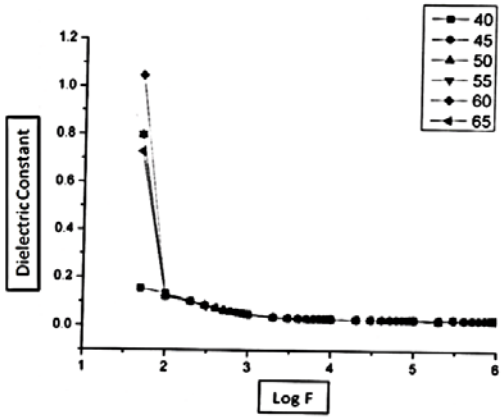

Figure 3.3: Variation of Dielectric Constant with Log f

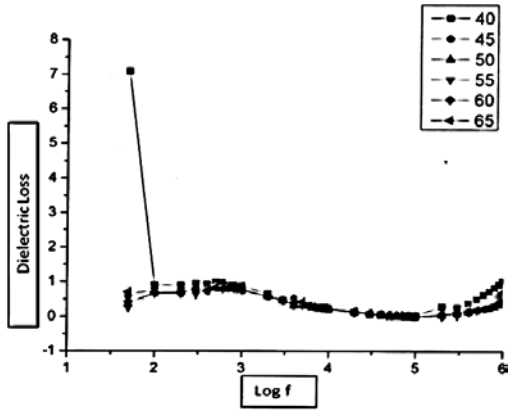

Figure 3.4: Variation of Dielectric loss with Log f

4. Conclusion

The powder X-ray diffraction studies confirm the crystalline perfection of the grown L-PCCM single crystal. The grown crystal was characterized by single crystal XRD and confirmed that the crystal belongs to orthorhombic crystal system with lattice parameter P. The optical absorption study shows that L-PCCM was optically transparent in the entire visible and near IR region with a lower cut-off wavelength that 230 nm. The FT-IR spectrum reveals the mode of vibrations of different molecular groups present in the title compound. The characteristics of low dielectric loss for the sample suggest that it possesses enhanced optical quality with lesser defects and this parameter is of vital significance for nonlinear optical applications.

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