International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064, Impact Factor (2013): 4.438
www.ijsr.net

Synthesis, Growth and Characterization of Nonlinear Optical L-Proline Cadmium Chloride Single Crystal

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Abstract: ***A good quality of L-proline cadmium chloride single crystal was grown by a slow evaporation technique. Single crystal XRD analysis reveals that LPCC crystal belongs to orthorhombic system with space group of $P2_12_12_1$. The transparent nature of the LPCC crystal was confirmed from the UV- VIS-NIR spectrum. The functional group was confirmed by FTIR. Mechanical behavior has been studied by Vickers microhardness test.***

Keywords: Semi organic, Nonlinear optical, LPCC, Spectroscopy.

1. Introduction

Nonlinear optical materials have attracted many researchers because of their potential applications in optical modulations, optical switching, optical logic, laser technology, frequency conversion, optical data storage for the developing technologies in telecommunications and signal processing [1-3, 6,7]. In general, amino acids act as both an acceptor and donor i.e. through proton donating carboxyl (-COOH) and proton accepting amino ($-NH_2$) groups [6]. L- Proline Cadmium Chloride is a semi-organic material crystallizing in the crystal form of orthorhombic crystal system with space group $P2_12_12_1$ [1]. In this paper, we report on the growth and characterization of semiorganic L- Proline Cadmium Chloride (LPCC) single crystal. The L- Proline Cadmium Chloride was grown by a slow evaporation method at room temperature. The grown crystal was subjected to various characterizations such as single crystal XRD study to understand the crystal system and space group and UV-vis-NIR, Fourier transform infrared (FTIR) absorption and microhardness to study its pertinent characterisitcs.

2. Experimental

2.1 Synthesis And Crystal Growth

L- Proline Cadmium Chloride was synthesized by taking L-Proline and Cadmium Chloride in the stoichiometric ratio of 1:1 in the aqueous solution by slow evaporation method. The required amount of starting materials for the synthesis of LPCC was calculated according to the reaction.

$$CdCl_2.H_2O + NH_2CH_2CH_2CH_2CHCOOH \rightarrow Cd(NH_2CH_2CH_2CH_2CHCOOH)Cl_2.H_2O$$

The calculated amount of L- Proline was first dissolved in double distilled water. Cadmium Chloride was then added to the L- Proline solution by stirring for 3 hours. The prepared solution was filtered using filter paper so that all the impurities could be removed. The filtered solution was allowed to evaporate at room temperature. After a period of 20 – 25 days, single crystal of LPCC was harvested successfully. Fig 1. shows as-grown crystal of LPCC.

Figure 1: Photograph of LPCC Crystal

3. Results and Discussion

3.1 Single crystal X-ray diffraction analysis

Single crystal XRD study reveals that LPCC crystal belongs to orthorhombic system with space group of $P2_12_12_1$. The cell parameters of L-PCC crystal are a= 7.325 Å, b=10.025 Å, c =13.554 Å, α=9 0°, β=90°, γ=90°and volume = 992Å ^{3}. The obtained data are found to be in good agreement with the reported values [7].

3.2 Uv-Vis Spectroscopy

A good optical transmission is desirable for NLO crystal. To determine the optical transmittance range and hence the suitability for the application of optical device, the grown crystal was analyzed by UV-VIS spectral analysis. The UV-spectrum is recorded in the wavelength range of 200-1100 nm and it is shown in fig 2. The crystal shows good transmittance in the entire visible region. As observed in the spectrum, there is no significant absorption in the range 300-800 nm hence the crystal can be used for NLO application. The cutoff wavelength for the crystal is about 328 nm.

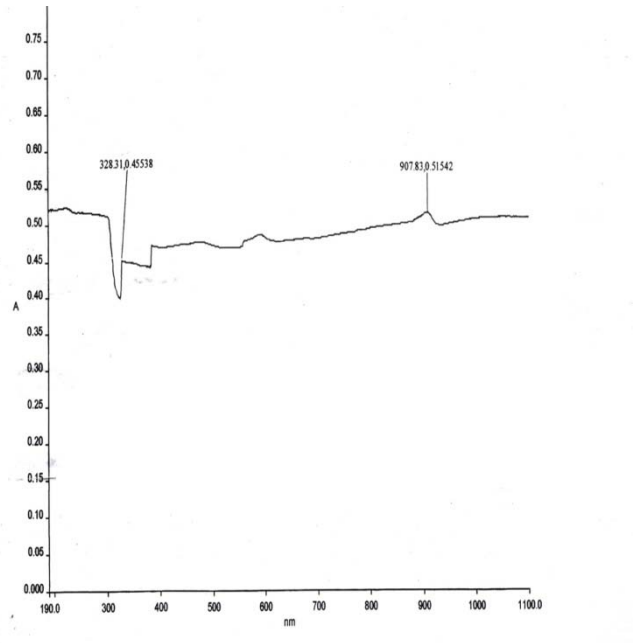

Figure 2: UV-VIS spectrum of LPCC single crystal

3.3 Fourier Transform Infrared (FTIR) Analysis

FTIR spectrum of LPCC crystal was recorded in the range of 400-4000 cm^{-1}. The obtained FTIR spectrum is shown in fig. 3 and the nature of chemical bonding between different functional groups are tabulated and given in table 1.

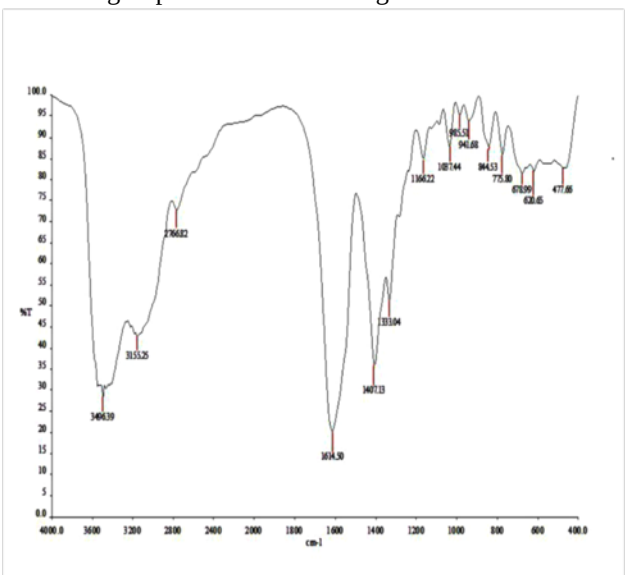

Figure 3: FT-IR spectrum of L-PCC

Assignments	Wave number cm^{-1}
Stretching vibration of H_2O molecule	3496.39
N-H Stretching vibration	3155.25
N-H Stretching vibration	2766.82
NH_2^+ in plane deformation	1614.50
COO^- Symmetric Stretching	1407.13
Wagging CH_2^+	1333.04
Twisting NH_2^+	1166.22
C- N Stretching	1037.44
Rocking CH_2	985.51
Rocking CH_2	941.68
Rocking CH_2	884.53
In- plane deformation of COO^-	775.80
In- plane deformation of $CONH_2$	678.99
Wagging COO^-	620.65
Rocking COO^-	477.66

The peak appearing at 3496 cm^{-1} was assigned to the Ostretching vibration of H_2O. The peaks for the N-H stretching vibration were observed at 3155 cm^{-1} and 2766 cm^{-1}. The peakfor the COO^- Symmetric Stretching was observed at 1407 cm^{-1}. The plane deformations of COO^- were seen at 775 cm^{-1}, $CONH_2$ at 678 cm^{-1} and NH_2^+ at 1614 cm^{-1}. The observed peaks at 985, 941 and 884 were assigned to rocking modes of CH_2. The C-N stretching vibration was observed at 1037 cm^{-1}. The wagging mode of COO^- and CH_2^+ was observed at 620 cm^{-1} and 1333 cm^{-1} [5,8,9].

3.4 Vickers microhardness test

Analysis of mechanical properties of the grown crystal is also important for the fabrication of electronic and optical devices. Micro hardness studies have been carried out on a selected well transparent single crystal using micro hardness tester, filtered with a Vickers diamond pyramidal indenter. To get accurate results of hardness if the grown crystal indentations well made on the LPCC crystals with applied load ranging from 25g to 100g. The values of Vickers micro hardness at different loads were calculated using the relation:

$$\mathbf{H_V = 1.8544 \frac{P}{d^2}\ kg\ mm^{-2}}$$

Where P is the applied load and d is the mean diagonal length of the indenter impression.

Figure 4 shows the variation of hardness with the applied load. It is observed that the hardness of LPCC increases by increasing load.

The plot of log P against log d is shown in Fig 5 is a straight line which is in good agreement with Mayer's law. The slope of the graph gives 'n' and it is determined to be 3.589. 'n' should be between 1 and 1.6 for hard materials and above 1.6 for softer ones. Hence LPCC belongs to soft material category.

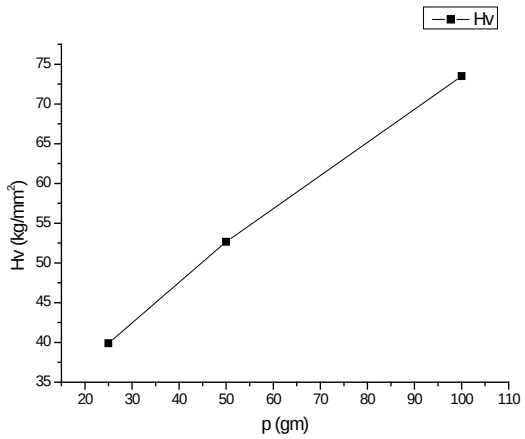

Figure 4: shows the variation of hardness with the applied load.

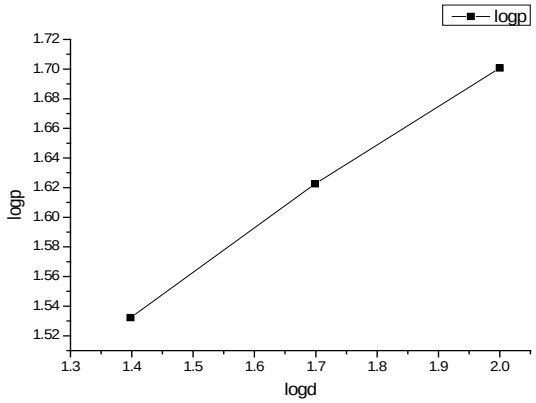

Figure 5: Graph between log *P* and log *d*.

4. Conclusion

A good quality of L-proline cadmium chloride single crystal was grown by a slow evaporation technique. Single crystal XRD analysis reveals that LPCC crystal belongs to orthorhombic system with space group of $P2_12_12_1$. The transparent nature of the LPCC crystal was confirmed from the UV- VIS-NIR spectrum. The functional group was confirmed by FTIR. Mechanical behavior has been studied by Vickers microhardness test.

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