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Growth, structural and spectral properties of L-Alanine Cadmium Chloride single crystal

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Abstract : Single crystals of L-Alanine Cadmium Chloride (LACC), an organometallic nonlinear optical material, have been grown by the slow evaporation technique. The grown crystals were subjected to various characterization techniques such as single crystal and powder XRD, FTIR and UV-VIS. Second harmonic generation was confirmed by the Kurtz and Perry powder technique. Electrical parameters such as dielectric constant, dielectric loss, also have been studied. The low dielectric constant and dielectric loss suggest that this material is a good candidate for microelectronic applications.

Keywords : LACC, XRD, FTIR, Uv-Vis-NIR, Nonlinear Optical.

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1. Introduction

The overwhelming success of molecular engineering in controlling non-linear optical (NLO) properties has attracted the attention of researchers to search for a variety of new types of NLO materials [1,2]. However the implementation of single crystals of organic materials in practical device-applications has been impeded by their inadequate transparency, poor optical quality and low LASER threshold. Inorganic crystals have excellent mechanical and thermal properties, but they possess relatively modest non-linearity because of the lackof π electron delocalization. Hence recent search is concentrated on organometallic materials due to their large nonlinearity, high resistance to LASER induced damage, low angular sensitivity and good mechanical hardness [3,4]. Now a day the organic and inorganic materials are being replaced by semiorganic materials because they share the properties of both organic and inorganic materials. Also the semiorganic materials show large nonlinearity, low angular sensitivity and good mechanical hardness. In our present work the single crystals of LACC were grown by slow evaporation technique and its solubility was determined. Again the results of single crystal and powder XRD analyses, FTIR, UV-VIS, TGA-DTA, SHG, Vickers microhardness and electrical studies of the grown crystals are reported.

2. Experimental

LACC was synthesized from L-alanine and cadmium chloride monohydrate taken in the equimolar ratio. An adduct was formed according to the following reaction:

$CH_3CHNH_2COOH + CdCl_2 \Rightarrow CH_3CHNH_2COOH.CdCl_2$

Well defined single crystals (size up to 12 x 7 x 2 mm^3) of good transparency were collected in four weeks.

3. Result and Discussion

The powder XRD pattern of LACC is shown in Figure 1, which consists of peaks corresponds to pure LACC and no other peaks of other phase or element is detected, with in the detection limit of the instrument. The unit cell dimensions calculated from the powder XRD data are a =16.275 (± .002) Å, b =7.265 (± .002) Å and c =7.97 (± .002) Å. It agrees with the reported values [5].

Figure 2 shows the FTIR spectrum of LACC. The NH_2 group of L-alanine is protonated by the COOH group, giving rise to NH^{3+} and COO^- groups. The broad envelope in the higher energy region 3044 to 3250 cm^{-1} and 3425 to 3500 cm^{-1} is due to NH^{3+} symmetric, asymmetric stretching vibrations and the absorption peak at 1616 cm^{-1} is assigned to NH^{3+} bending degenerate mode.

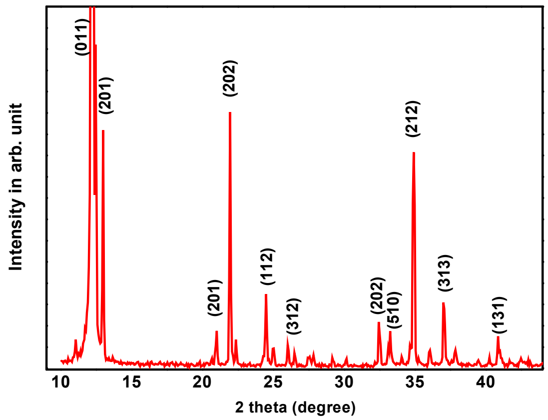

Figure 1: The powder X-ray diffraction pattern of L-alanine cadmium

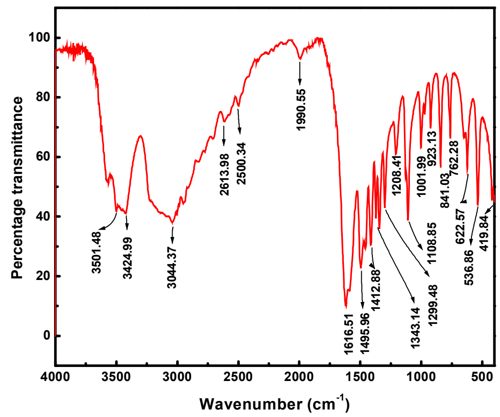

Figure 2: FT-IR spectrum of L-alanine cadmium chloride

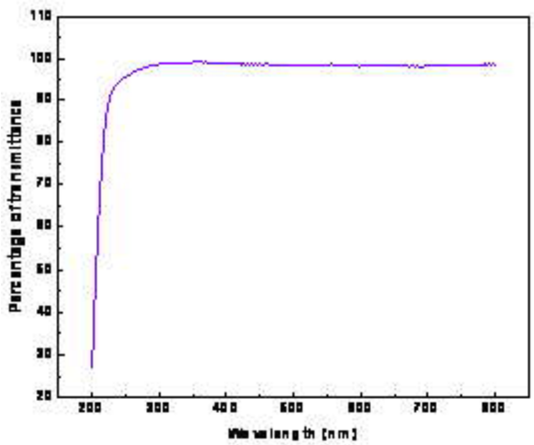

Figure 3 : The UV - VIS - NIR transmittance spectrum of L-alanine cadmium chloride showing the complete transmittance in the entire UV - VIS - NIR region.

The region of absorption bands from 3044 cm^{-1} to about 2500 cm^{-1} is due to multiple combinations of overtone bands, the strong absorption at 1412 cm^{-1} corresponds to COO^- symmetric stretch [16]. The COO^- bending and rocking frequencies occur in the normal positions at 762 cm^{-1}, 622 cm^{-1} and 536 cm^{-1}. Also the absorption at 1343 cm^{-1} and 1001cm^{-1} are due to CH_3 symmetric bending and rocking mode. The absorption peaks at 923 cm^{-1} and 841cm^{-1} are assigned to C-C-N symmetric stretching vibrations. These vibrations prove the presence of expected functional groups in the compound.

The UV-VIS –NIR transmittance spectrum of LACC is shown in Figure 3. It shows that there is no significant absorption in the range of 200 - 800 nm. This is the advantage of using the amino acids, where the absence of strongly conjugated bonds leads to wider transparency in the visible and UV spectral regions [8]. The lower cut at 200 nm along with good optical transparency enhances the usefulness of LACC for optoelectronic applications and it is an essential parameter for NLO applications. The NLO property of the crystal was confirmed by the Kurtz and Perry powder technique. The finely powdered sample was densely packed between two transparent glass slides. A fundamental laser beam of 1064 nm wavelength (8 ns pulse width with 10 Hz pulse rate) from an Nd-YAG LASER was made to fall normally on the sample cell. The power of the incident beam was measured using a power meter. The transmitted fundamental wave was passed over a monochromator which separates 532 nm (second harmonic signal) from 1064 nm and absorbed by a $CuSO_4$ solution which removes the 1064 nm light. The green light was detected by a photomultiplier tube and displayed on a storage oscilloscope. The KDP crystal was used as the reference material in the SHG measurement. The powder SHG efficiency of the crystal is compared with KDP and it is found to be 0.57 times that of KDP but 1.66 times greater than that of the parent material L-alanine.

4. CONCLUSION

The single crystals of organometallic L-Alanine Cadmium Chloride were grown by slow evaporation technique and characterized by X-ray diffraction studies. The FT-IR spectral analysis confirms the presence of functional groups in the compound. The material has good optical transparency in the entire visible region with a lower cut of wave length at 200 nm and the NLO property is confirmed by SHG measurement.

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