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Molecular Structure, First-order Hyperpolarizability Studies of L- Arginine Perchlorate

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Abstract : An organic nonlinear optical (NLO) material L-Arginine Perchlorate, was synthesized by slow evaporation technique. The synthesized material was purified by repeated recrystallization. The grown crystal was characterized by single crystal XRD, FT-IR and UV-Vis NIR techniques. The FT-IR spectrum was recorded for LAPCl crystal and the functional groups were identified. The assignments were made with the help of theoretical information obtained from the Density Functional theory. The first order hyperpolarazibility of LAPCl was also determined. The second harmonic generation (SHG) from the material was confirmed using Nd:YAG laser.

Keywords : Nonlinear Optical, Fourier transform infrared spectroscopy, Uv-Vis-NIR) Second harmonic generation, LAPCL

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1. Introduction

In recent years the need for nonlinear optical materials is much more than other materials because of their significant impact on laser technology, optical communication and optical data storage technology [1]. Organic crystals with large nonlinear optical (NLO) effects make them attractive for applications in frequency conversion and optical processing [2, 3]. The importance of amino acids in NLO applications is due to the fact that all the amino acids have chiral symmetry and crystallize in noncentro- symmetric space groups [4]. Many number of natural amino acids are individually exhibiting the nonlinear optical properties because they are

characterized by chiral carbons, a proton-donating carboxyl (-COOH) group and the proton-accepting amino (-NH2) group. Thus L-arginine, L- histidine and L-alanine have been exploited for the formation of salts with different organic/inorganic acids. In our present work L- Arginine Perchlorate was grown successfully and characterized.

2. Synthesis and Characterization:

2.1 Synthesis

LARPCL was synthesized from high purity L-arginine (Merck-99 %) and perchloric acid (Merck-70 %) taken in equimolar ratio. The stoichiometric amounts of the reactants were thoroughly dissolved in deionized water. The reaction involved in the synthesis is as follows :

$$NH_2\,CNHNH\,(CH_2)_3\,CH\,NH_2COOH + HClO_4 \longrightarrow NH_2\,CNH_2^{+}\,NH\,(CH_2)_3\,CHNH_3^{+}COO^{-}.\,ClO_4^{-}$$

The synthesized material was then purified from aqueous solution by recrystallization process.

2.2 Single crystal XRD

In order to obtain the crystal data of LARPCL crystals, single crystal X-ray diffraction studies were carried out using ENRAF NONIUS CAD4-F single crystal X-ray diffractometer with MoK_α (λ= 0.71073 Å) radiation. The single crystal XRD data of LARPCL crystal indicates that it crystallizes in orthorhombic system with $P2_12_12_1$ space group.

2.3 FTIR spectral analysis

Figure 1 shows the infrared spectrum of LARPCL recorded in the range 4000 – 400 cm^{-1} using the Bruker IFS 66V FT-IR spectrometer by potassium bromide pellet technique to confirm the presence of functional groups. It is noted from the spectrum that the bands at 3476 and 3403 cm^{-1} evidence the presence of weakly hydrogen bonded N-H groups. The band at 3277 cm^{-1} corresponds to stronger hydrogen bonded N-H groups. The bands at 3062, 2973 2946, 2881, and 2830 cm^{-1} relate to stretching vibrations of C-H bonds of CH and CH_2 groups. The intense band comprising of peaks near 1636 cm^{-1} may be assigned to asymmetric

stretching of COO^{-}, asymmetric bending of NH_3^+ and NH_2 bending vibrations. The symmetric bending vibrations of NH_3^+ and COOH groups are positioned at 1490 and 1423 cm^1.

2.4 Optical transmittance and nonlinear optical studies

The optical transmission spectrum of LAPCl single crystal was recorded in the wavelength region of 200-2000 nm using VARIAN CARY 5E spectrometer. The spectrum of LArM crystal is shown in Figure 2. It is evident that the crystal possesses a wide optical transparency window from 390 -1100 nm. It is also clearly indicates that the UV cut-off wavelength lies at 390 nm. The presence of low cut-off wavelength and the wide optical transmission window are the suitable parameters for frequency doubling of laser radiation.

2.5 Hyperpolarizability Calculations

The first-order hyperpolarizibility (β_{ijk}) of the novel molecular system of LAPCl was calculated. Hyperpolarizibility is a third rank tensor and strongly depends on the method and basis set used. The calculated first order hyper polarizability (β_{total}) of LAPCL is 2.7524 x10^{-30} esu.

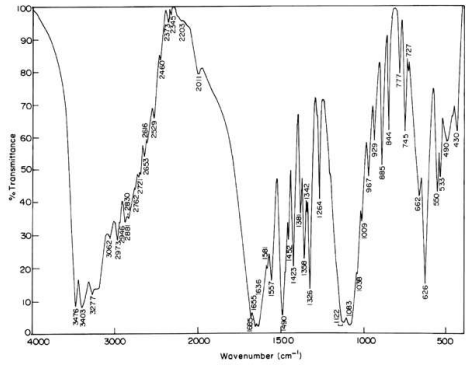

Figure 1. FT-IR spectrum of LARPCL

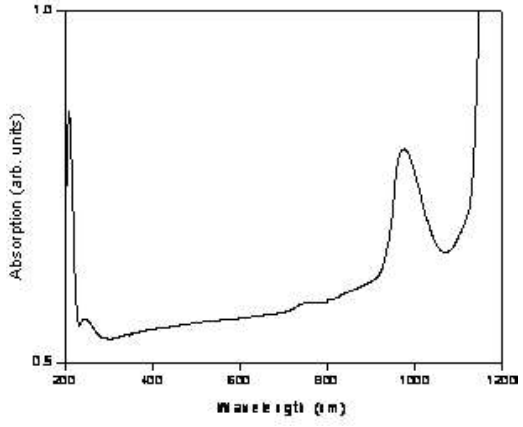

Figure 2. Optical absorption spectrum of LArM

3. Conclusion

Single crystals of LAPCl are conveniently grown by employing slow evaporation technique. XRD studies confirm the structure of grown crystals. The optical absorption spectrum of LArM confirms that the crystals possess higher percentage of transmission over a wide range from 390 -1100 nm. SHG in the crystal was confirmed by NLO test.

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