

OPTICAL ABSORPTION SPECTRUM AND STRUCTURAL ANALYSIS OF L-ORNITHINE MONOHYDROCHLORIDE

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Abstract

The structure of the molecule was optimized by single crystal X-ray diffraction using BRUKER NONIUS CAD 4 single crystal X-ray diffractometer with Cu K α radiation. Powder XRD pattern was compared with simulated both coincide with each. UV-visible spectrum of the compound was recorded in the region 200–1200 nm. From X-ray analysis crystal parameters were identified and Energy gap was found to be 5.08 eV.

Key Words: UV-visible, LOMHCL, XRD

INTRODUCTION

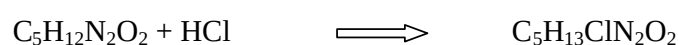
Organic nonlinear optical (NLO) materials because of their wide transparency in UV and visible region, high nonlinear susceptibility, high laser damage threshold and fast response than the commercially available inorganic materials[1-5]. By molecular engineering, one can develop many organic crystals displaying better NLO properties than the inorganic materials, in particular for second harmonic generation (Senthil S., et al 2009). Molecules allow strong π - π^* and σ - σ^* transition in the UV-vis region with high extinction coefficients (M. Karabacak 2012)[6-12]. This chapter deals with the experimental and theoretical investigation of L-Ornithine Monohydrochloride (LOMHCL) single crystal.

EXPERIMENTAL DETAILS

Synthesis

Single crystal of LOMHCL was synthesized by dissolving stoichiometric amount of L-Ornithine (Merck 99%) and high purity hydrochloric acid in deionized water[13-18].

The chemical reaction that takes place in this process is as follows



Characterization

The grown crystal was subjected to single crystal X-ray diffraction study at room temperature using BRUKER NONIUS CAD 4 single crystal X-ray diffractometer with Cu K α radiation[19-25]. The crystals were also subjected to powder X-ray diffraction analysis. A Rich-Seifert powder X-ray diffractometer with CuK α radiation ($\lambda = 1.5418 \text{ \AA}$) was used at a scan speed of $0.02^\circ/\text{s}$ [26-31]. The absorption spectrum for the specimen was recorded using a Varian Cary 5E UV-Vis-NIR spectrometer in the region 200 – 1200 nm.

RESULTS AND DISCUSSION

X-ray diffraction analysis

From the single crystal analysis it was observed that the crystal belongs to monoclinic crystal system having non-centrosymmetry[32-39], with P12₁1 space group. The crystal data and structural refinement data are given in Table 1. Experimental Powder XRD pattern is shown in Figure 1. Theoretically Simulated XRD pattern of

LOMHCL single crystal with indexed peak is also given in Figure 2. Both XRD patterns are almost similar in comparison.

Table 1 Crystal parameters of LOMHCL

Empirical Formula	$C_5H_{13}N_2O_2Cl$	
Formula weight	168.62	
Wave length	0.154180 nm	
Crystal system, Space group	Monoclinic $P12_11$	
Unit cell dimensions	$a = 9.9480(2)$ $b = 7.9637(2)$ $c = 4.9826(10)$	$\alpha=\gamma=90^\circ$ $\beta = 83.130^\circ(10)$
Cell volume	391.91(2)	
Calculated Density	1.4290 g/cm ³	
Absorption coefficient	0.433 mm ⁻¹	
F(000)	180	
Crystal size	0.71×.63×.24 mm ³	
Theta range for data collection	3.2774 to 52.7059 deg	
Limiting indices	-22≤h≤22;-17≤ k ≤ 17 ; -11≤ l≤11	
Reflections collected/unique	8892/8123	
Completeness to theta = 67.92	97.5%	
Refinement method	Full- matrix least squares on F ²	
Data/restraints/parameters	8123/0/103	
Goodness- of – fit on F ²	1.7983	

Final R indices [$I > 2\sigma(I)$] 80	$R_1 = 0.0157$; $WR_2 = 0.0089$
R indices (all data)	$R_1 = 0.0136$; $WR_2 = 0.0091$

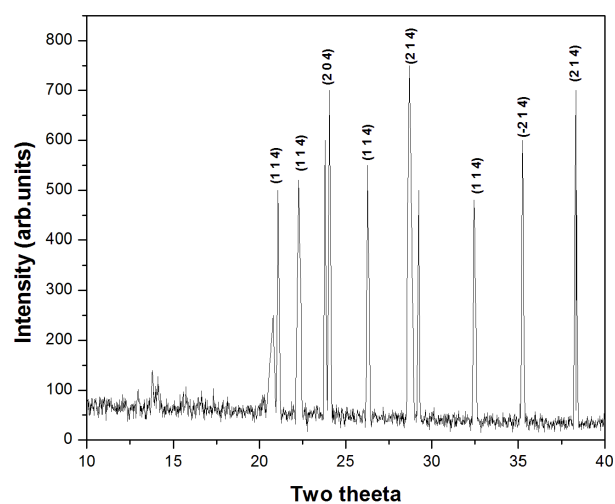


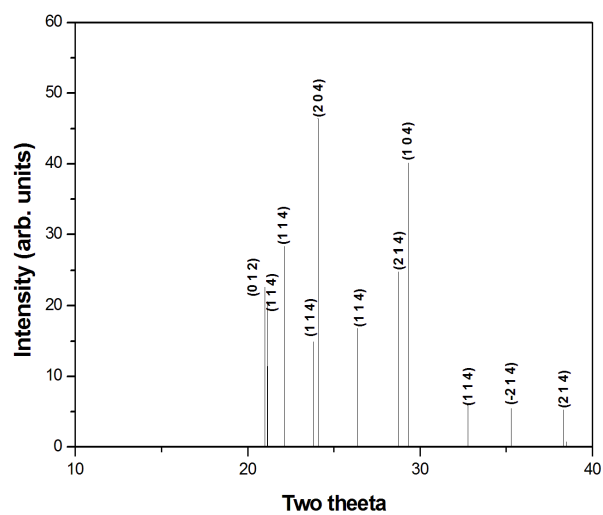
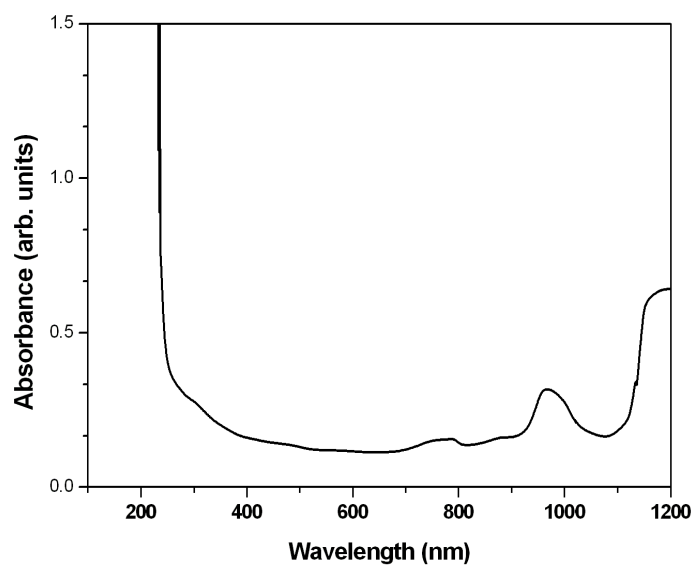
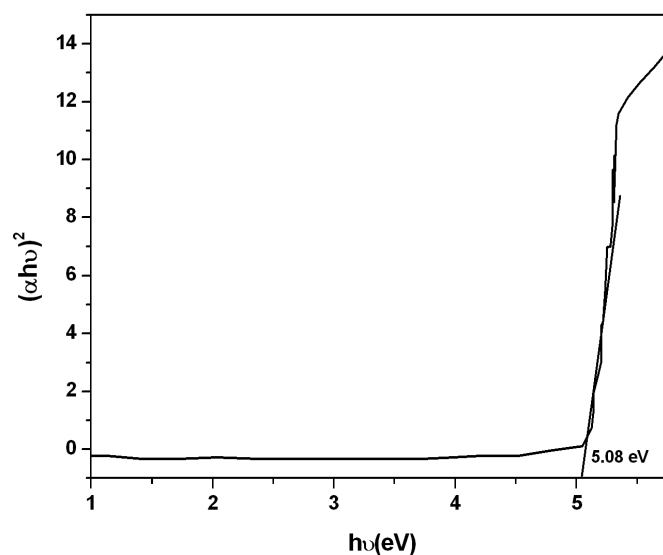
Fig. 1 Powder XRD spectrum of LOMHCL crystal**Fig 2 Theoretically simulated powder XRD pattern of LOMHCL**

Fig 3 Optical absorption spectrum of LOMHCL crystal**Fig 4 Optical band gap of LOMHCL crystal****Optical absorption spectrum**

The recorded UV-Vis-NIR spectrum is shown in figure 3. The crystal has sufficient transmission in the entire UV, visible and near IR region. The lower cut off wavelength for LOMHCL is around 250 nm[40-45]. The transmittance window in the visible region and near IR region enables good optical transmission of the second harmonic frequencies of Nd:YAG lasers. From the absorbance spectrum the band gap was evaluated. The E_g could be estimated from the plots of $h\nu$ versus $(\alpha h\nu)^2$. A plot of $h\nu$ versus $(\alpha h\nu)^2$ was drawn (figure 4) and the optical band gap (E_g) (Madhavan J 2007)

value was obtained from the interception of the linear portion of the curve with X-axis.

This gives the E_g values of 5.08 eV for LOMHCL crystal.

CONCLUSION

Optically transparent Prismatic single crystal of LOMHCL is grown by slow evaporation technique in a period of 40 days. The grown crystal was confirmed by x-ray analysis. The lower cut off wavelength of LOMHCL at 250 nm, recommends this material is a potential candidate for frequency doubling. Thus, the promising crystal growth characteristics and good optical properties make LOMHCL a potential material for photonics device applications.

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