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Growth and Z - Scan Characterization of L-ornithine Monohydrochloride

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A B S T R A C T

An efficient nonlinear optical material L-Ornithine monohydrochloride (LOMHCl) was well synthesized and harvested by low temperature slow evaporation method. The single crystal X- ray diffraction analysis confirms that the crystal belongs to monoclinic system with a space group of P21.The existence of third order nonlinear optical measurements were studied from Z- scan analysis. The closed and open aperture curve from the Z-scan shows negative nonlinearity and self-defocussing nature reveals it as an efficient nonlinear optical material for device fabrication.

***Key words*:** Crystal growth, Nonlinear optical material, Optical analysis, Z- Scan

Materials which show noticeable conversion capability for the development of second harmonic generation and its widespread transparency in ultraviolet and visible region are the essential aspects in the domain of optical applications [1]. The advancement of research in the field of nonlinear optics (NLO) is very much connected to the fast scientific method that occurred in interrelated fields for instance ultra-fast phenomena, optical communication and storage devices [2]. The optical response about an effective nonlinear optical sample assessed jointly by the chemical purity and structure composition. A moment ago, actions and happening on research display attention on establishing exceedingly competent nonlinear optical semi organic materials [3]. A nonlinear optical phenomenon creates the microscopic level view in a dielectric matter towards the electric field present in a potent energetic beam of light. The ray of light propagating through a dielectric emphasis change in the temporal and spatial distribution of charges for the reason that the electrons present in the atoms act together with the electromagnetic field existing in the light beam.

The importance of amino acid in the field of nonlinear optical application is clear from the point that majority of the amino acids crystallizes in acentric space group and possess asymmetric carbon atom. The dipolar nature displays unique chemical and physical features in amino acids, therefore making them an outstanding candidate in nonlinear optics. The crystal structure of the title compound already has been elucidated by Chiba *et al*. [4]. The synthesis, growth, spectral, dielectric, linear and nonlinear optical properties of L-Ornithine hydrochloride, was also grown using water and DMF as a solvent [5]. In this view point, the present work signifies the detailed report on the synthesis of a good quality efficacious semi organic L-Ornithine monohydrochloride by the scheme of slow evaporation in which nonlinearity is added favorable and prominent for NLO applications.

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MATERIALS AND METHODS

Material synthesis

The low temperature slow evaporation method was chosen to grow L-ornithine monohydrochloride (LOMHCl). The calculated amount of LOMHCl was taken and the required material was thoroughly dissolved in deionized water and DMF at a temperature of 40°C. The solution was stirred well using magnetic stirrer for 6 hours to ensure clear transparent solution. The saturated homogenous solution was filtered and was covered and kept in a room temperature. A color less transparent crystal was harvested in a growth period of3 weeks. The purity of the material was further increased by repeated recrystallization and the photograph of the grown crystal is shown in (Fig 1).

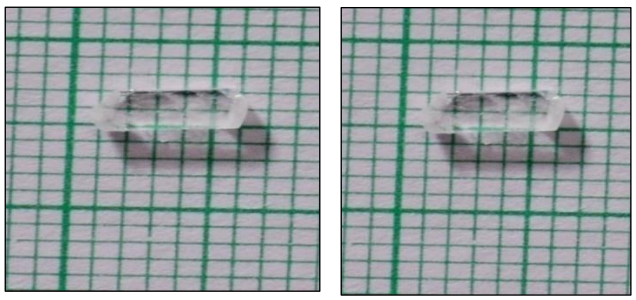

Fig 1 Single crystal of LOMHCl

RESULTS AND DISCUSSION

Single crystal diffraction analysis

Single crystal XRD discloses the lattice parameters as a =10.06Å, b= 8.05 Å, c=5.03Å, α = γ = 90˚, β = 96.93˚ and volume V= 404 Å^3. LOMHCl corresponds to the crystal system of monoclinic with $P2_1$ as space group and are in accordance with the previously reported value (Chiba *et al.* 1967) and is listed in (Table 1).

Table 1 Single crystal XRD crystallographic data of LOMHCl

Cell parameters	Present work	Reported work
Space group	$P2_1$	$P2_1$
a (Å)	10.06	10.005
b (Å)	8.05	7.992
c (Å)	5.03	5.000
α (˚), γ (˚)	90	90
β (˚)	96.93˚	96.98˚
Volume (Å^3)	404	396.83
System	Monoclinic	Monoclinic

Solubility test

The solubility of LOMHCl was determined for five different temperatures viz., 30˚ C, 35˚ C, 40˚ C, 45˚ C, 50˚ C. The solubility at 30˚ C was determined by dissolving LOMHCl salt in the solvent (water and DMF) taken in an air tight container maintained at this temperature with continuous stirring. After attaining saturation, the equilibrium concentration of the solute was estimated gravimetrically. The same procedure was repeated to estimate the solubility at different temperatures of LOMHCl solution is shown in (Fig 2). The LOMHCl exhibits positive coefficient of solubility and the solubility increases linearly with temperature.

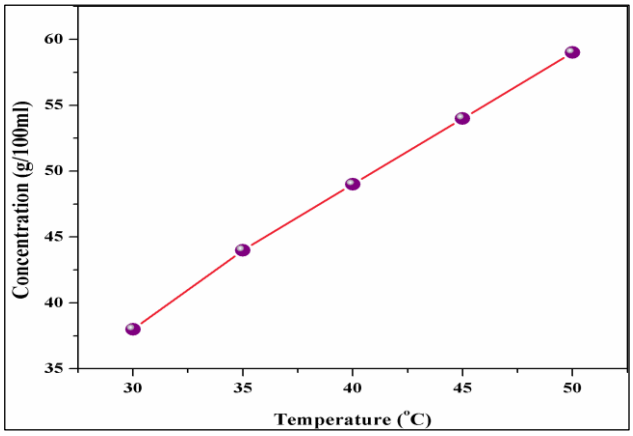

Fig 2 Solubility of LOMHCl

Estimation of plasma energy, penn gap energy, fermi energy and polarizability

The electronic polarizability (α) shows an important role in determine the efficacy of nonlinear effects of the materials. The electro optic polarizability of the material depends on the solid state parameters that serves as an competent approving methodin estimating nonlinear optical characteristics [6]. The dielectric permittivity of the crystal depends on the valence electrons present in the material.

The density (ρ) can be found out using the formula:

$$\rho = \frac{MZ}{N_A V} \ldots\ldots\ldots (1)$$

M is the molecular weight (168.62 g mol^{-1}), Z =2 be the total number of atoms per unit cell, $N_A$be the Avagadro number (6.023 x 10^{23}) and V the volume of unit cell. The calculated density was found to be 1.429 g/cm^3.

The valence electron plasma energy $\hbar\omega_p$is calculated as:

$$\hbar\omega = 28.8 \left(\frac{Z'*\rho}{M}\right)^{½} \ldots\ldots\ldots\ldots (2)$$

The sum of valence electrons Z' for LOMHCl is100. The dielectric permittivity was calculated to be 10.82.

$$\text{Penn gap Energy, } E_p = \frac{\hbar\omega p}{(\varepsilon-1)^{1/2}} \ldots\ldots\ldots\ldots\ldots (3)$$

$$\text{Fermi energy, } E_F = 0.2948\ \hbar\omega p^{4/3} \ldots\ldots\ldots\ldots (4)$$

From Clausius-Mosotti equation,polarisability(α_p) can be calculated as:

$$\alpha_p = \frac{3M}{4\pi N\rho} * \frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 2} \ldots\ldots\ldots (5)$$

The electronic polarizabilty due to band gap Eg is given as:

$$\alpha = \left[1 - \frac{\sqrt{E_g}}{4.06}\right] * \frac{M}{\rho} * 0.396 * 10^{-24} cm^3 \ldots\ldots\ldots\ldots (6)$$

Using the above equations, solid state parameters are estimatedthat serves as a supporting factor for nonlinear efficiency of a crystal [6].The calculated electrical criteria of LOMHCl are listed in (Table 2).

Table 2 Calculated parameters of LOMHCl

Solid state parameters	Calculated Values	Values of KDP
Plasma Energy (eV)	20.876 eV	17.28
Penn gap energy (eV)	6.661 eV	2.37
Fermi Energy (eV)	16.945 eV	12.02
Polarizability by Clausius Mosssoti relation	3.584*10^{-23}cm^3	2.10*10^{-23}cm^3

Determination of non-linear optical studies

The NLO is an important parameter for organic, inorganic and semi-organic materials to show its optical alertness in the domain of photonics, optoelectronics, communications(optical), laser development, etc. The grown LOMHCl was thoroughly analysed to undergo second harmonic generation process by the Kurtz–Perry method [7]. The material was finely powdered and a high beam Nd-YAG laser (1064 nm) made to pass through the material with sample material as KDP. The SHG output shows green light emission.

The nonlinear property of the material was proved by extending LOMHCl to third order harmonic generation studies (Z-scan). This was employed using Nd-YAG laser (Coherentcompass TM215M-50) with 532 nm to show third order nonlinearities. The Z-scan method is an accurate and simple method for determining nonlinear absorption and refraction to prove the nonlinearity of the compound. The result verifies better nonlinear optical characteristics and its nonlinear absorption and refraction are dispensed to the negative non linearity and the two-photon absorption process. The change in the refractive index with the rise in temperature leads to self-defocusing nature, which shows evidence from the negative nonlinear variation. The closed aperture configuration is gentler in yielding nonlinear absorption and refraction. The observed peak followed by the valley configuration in Figure 3a illustrates the negative nonlinearity, which is attributed to self-defocusing nature [8]. In the open aperture configuration, the

transmittance curve shown in (Fig 3b) is symmetric with respect to focus and shows the two-photon absorption process. This shows its efficiency over possible recognition of signal processing devices in optics.

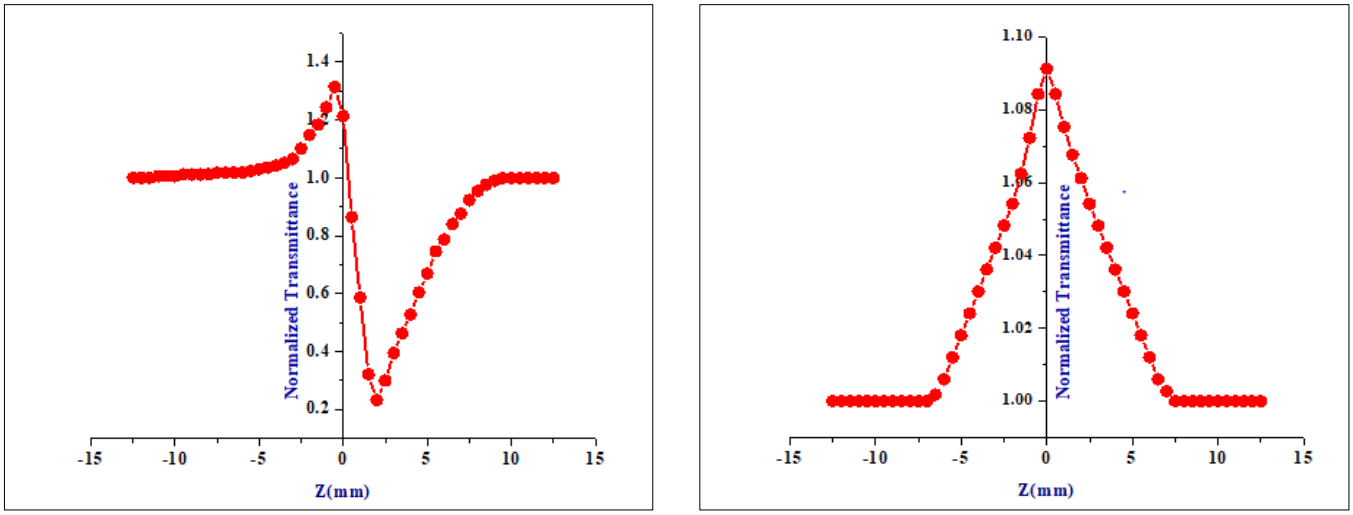

Fig 3 a,b Closed and open aperture of LOMHCl

Hence, the nonlinear refractive index (n2) and (β) was calculated to be 5.252 x 10^{-8}cm2/W and 0.07 x 10^{-4} cm/Wcm/W respectively. The absolute susceptibility |χ(3)| was identified to be 3.658 x 10^{-6}esu. This was clearly and elaborately reported in our previous work [5].

CONCLUSION

LOMHCl was grown successfully by slow evaporation method. The cell parameters of the grown crystal was elucidated through single crystal XRD. The monoclinic crystalline nature was confirmed from single crystal XRD.Z – Scan study reveals third order nonlinear nature of the grown LOMHCl. The results from various characterizations highlights that LOMHCl is a potential material for photonic device fabrication.

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