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Growth and Characterization of L-Ormithine Monohydrochloride doped Hippuric Acid Single Crytals for NLO Applications

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Abstract

In the current study, L-ornithine monohydrochloride added Hippuric acid LOMHA single crystals are synthesized successfully by utilizing slow evaporation solution technique (SEST). The obtained crystals are belonging to the orthorhombic system confirmed by single crystal X-ray diffraction technique (SXRD). The crystalline nature and purity of LOMHA crystal was confirmed by powder XRD pattern. The chemical composition is resolved by the Fourier transform infrared (FTIR) spectroscopy and energy dispersive X-ray analysis. The UV-Visible spectroscopic study showed that the lower cut-off wavelength was found to be 227.82 nm it indicated the good transmission of crystal. The dielectric study emphasizes that the LOMHA crystal is good in the applicability for NLO device applications. The grown crystals showed improvement in the thermal stability upon doping of LOMHA. SHG efficiency of HA is increased relatively upon the inclusion of LOM. These results favor the competency of LOM doped HA crystal in various NLO and laser assisted applications.

Keywords: Slow evaporation method, XRD, FTIR, UV-Visible, Dielectric constant, SHG.

1. Introduction

In the development of device fabrication, nonlinear optical (NLO) crystals are much concentrating materials in various industries viz., the optoelectronic and photonic fields, and fiber optical communication industry [1]. The symmetrical or regular arrangement of atoms in crystalline lattice point is called crystal. The crystals are used in many of places in our everyday life, chemical industries, food industries, purification technique, etc. In recent year science association of nonlinear optics developed in many applications [2]. The crystals it produced the nonlinear optical effect from electricity, magnetic field and strain field is called NLO crystals. The NLO crystal is formed in any kind of materials like Organic, inorganic and semiorganic crystals are used in the nonlinear optics [3]. Nonlinear optical (NLO) crystals are becoming more and more important materials in a variety of industries, including the photonic, fiber optic, and electronic sectors, as device production advances [4]. The intention is that these NLO materials regular periodic collections of atoms in their crystals allow them to have high levels of light transmission and the capacity to

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convert frequencies [5]. This indicates less light dispersion. NLO (Non-Linear Optical) crystals have been the subject matter of theoretical and experimental scrutinization during the past 20 years. L-ornithine monohydrochloride amino acids due to their significant impact as a dopant in improving the optical, thermal, mechanical, and SHG efficiency of hippuric acid crystals parameters that are crucial for NLO applications [6]. In the LOM molecule, the ornithine and chloride have cations and anion, respectively [7]. Due to LOM's zwitter ionic nature and significant dipole moment, it could be a useful dopant to improve the crystals performance of hippuric acid. The NLO crystal of L-ornithine monohydrochloride added Hippuric acid LOMHA single crystal is grown and its characterization investigations are single crystal XRD, Powder XRD, FTIR, UV-visible, Dielectric constant, TGA/DTA and SHG.

2. Experimental procedure

The L-ornithine monohydrochloride added Hippuric acid LOMHA single crystal was prepared by slow evaporation method. The calculated amount of main solvent Hippuric Acid was added into the beaker which containing acetone according to the solubility and stirred for 3 h. On the other side the calculated amount of dopant solvent LOM was added into the beaker which containing distilled water according to the solubility and stirred for 5 h. In order to obtain a homogeneous mixture, both solutions were mixed while being continuously stirred with a magnetic stirrer for 4 h. The LOM doped HA transparent solution was filtered with good quality filter paper. The good quality of LOMHA crystals obtained 37 days is shown Fig.1.

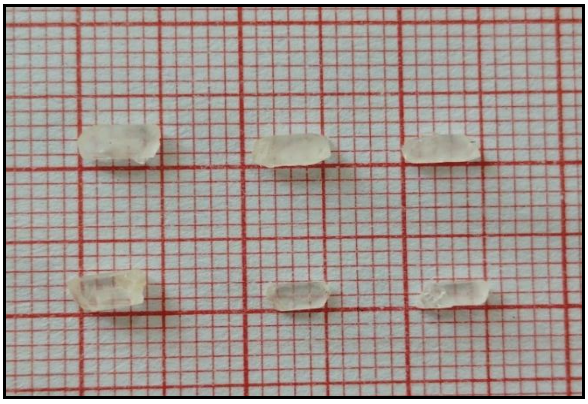

Fig.1 Grown single crystal of LOMHA

3. Characterization studies

3.1. Single crystal XRD

Table 1. STRUCTURE REFINEMENT DATA

Identification code	HLO_03_22022024
Chemical formula	$C_9H_7NO_3$
Formula weight	177.16 g/mol
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal size	0.666 x 0.760 x 0.824 mm
Crystal system	orthorhombic
Space group	$P_{21\ 21\ 21}$
Unit cell dimensions	a = 8.8828(3) Å
	b = 9.1173(3) Å
	c = 10.5829(4) Å
Volume	857.08(5) $Å^3$
Z	4
Density (calculated)	1.373 g/cm^3
Absorption coefficient	0.105 mm^{-1}
F(000)	368

Single-crystal X-ray Diffraction is a non-destructive analytical technique which provides detailed information about the internal lattice of crystalline substances, including unit cell dimensions, bond-lengths, bond-angles, and details of site-ordering [8]. The final cell constants of a = 8.8828(3) Å, b = 9.1173(3) Å, c = 10.5829(4) Å, volume = 857.08(5) Å3, are based upon the refinement of the XYZ-centroids of 4036 reflections above 20 σ(I) with 5.898° < 2θ < 56.15°. Data were corrected for absorption effects using the Multi-Scan method. The ratio of minimum to maximum apparent transmission was 0.781. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9180 and 0.9330.

3.2. Powder X-ray diffraction analysis

The powder X-ray diffraction is investigated and given crystallinity and analysis the lattice parameter [9]. L-Ornithine monohydrochloride doped Hippuric Acid crystal grown in acetone (LOMHA) was examined at a wide angle of 5° to 60° using a powder X-ray diffractometer. Fig. 2. represents the X-ray Diffraction for the sample LOMHA. LOMHA represents the diffraction peaks for the sample LOMHA are 12.96°, 16.22°, 16.69°, 19.31°, 19.91°, 21.69°, 23.38°, 27.91°, 28.80°, 30.46°, 31.60°, 32.70°, 34.61°, 35.33°, 40.45° and 43.84° corresponding to hkl values of (011), (111), (020), (120), (002), (012), (211), (202), (131), (310), (103), (-311), (041), (410) and (051) this crystalline planes confirms the orthorhombic crystal structure orientation with space group $P2_1 2_1 2_1$ which are referred from the JCPDS card no. (00-030-1748). Powder X-ray diffraction analysis was used to examine the crystalline quality and their cell dimensions. A Rigaku X-ray diffractometer with a Cukα radiation source (1.5406 Å) was utilized for this purpose. Using Bruker SHELXTL Software Package, the growing crystals lattice parameter values were computed and the peaks were indexed.

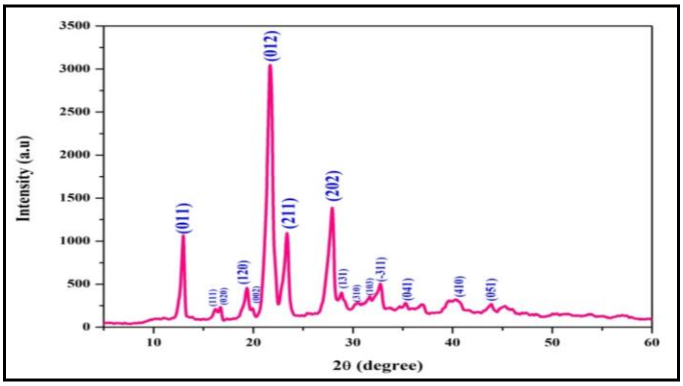

Fig 2. Powder XRD pattern of LOMHA

3.3. Fourier Transform Infrared (FT-IR) Analysis

The FT-IR of the L-Ornthine monohydrochloride doped Hippuric acid, recorded between 500 and 4000 cm^{-1} using KBr pellet Elmer RXI FTIR spectrometer, is displayed in Fig.3. Analysis was conducted to determine the molecular structure and chemical bonding of the material. For N-H stretching, the bond (alkyne group) at 3342 cm^{-1} is designated [10]. The frequency for C-N stretching is 3060 cm^{-1}. At 2691 cm^{-1} and 2478 cm^{-1}, the distinctive stretching vibrations of CH_2 stretching take place. The peak for C=O stretching is located at 1749 cm^{-1}. At 1553 cm^{-1}, the N-C-N asymmetric stretching vibration was seen. Asymmetric stretching vibration with C=S verified for 1403 cm^{-1} in doped crystal. The N-C-S symmetric bending is shown by the absorption band at 658 cm^{-1}. The cause of the frequency 723 cm^{-1} is symmetric stretching with C=S. The presence of dopant in the crystal is verified by FT-IR.

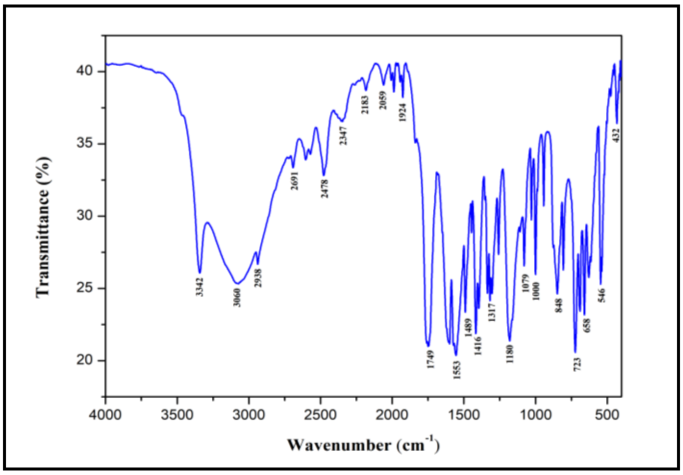

Fig 3. FT-IR spectral pattern of LOMHA

Table 2. FT-IR Assignments

Wavelength region(cm^{-1})	**Functional Group**
3342	N-H Stretching
3060	C-N Stretching
2691	CH_2 Stretching
2478	CH_2 Stretching
2347	Hydrogen bonding interaction of COOH in crystal lattice
1749	C=O Stretching
1553	N-C-N Stretching
1489-1416	C=S Asymmetric Stretching
1180	CH_2 Stretching
1079-1000	C-N Stretching of aliphatic amines present in hippuric acid
848	C-H Stretching
723	C=S Symmetric Stretching
658	N-C-S Symmetric Bending

3.4 UV Visible spectral analysis

One important NLO crystal parameter is optical transmittance. UV-Vis spectral analysis, sometimes referred to as UV-Vis or UV/Vis spectrophotometry, is a workhorse technique in analytical chemistry. Since the promotion of electrons in the s and π orbitals from the ground state to higher energy states occurs during the absorption of UV and visible light, the optical properties of the materials are significant because they reveal information about the electronic band structure, localized state, and type of optical transitions.

Grown crystals of 0.5 cm thickness were taken for the analysis. Using a Jasco V-570 UV-VIS-NIR spectrophotometer, the transmission and absorption spectra in the 200–800 nm wavelength range were captured [11].

$$\mathbf{A = 2\text{-}logT}$$

Where, A is Absorbance and T is Transmittance

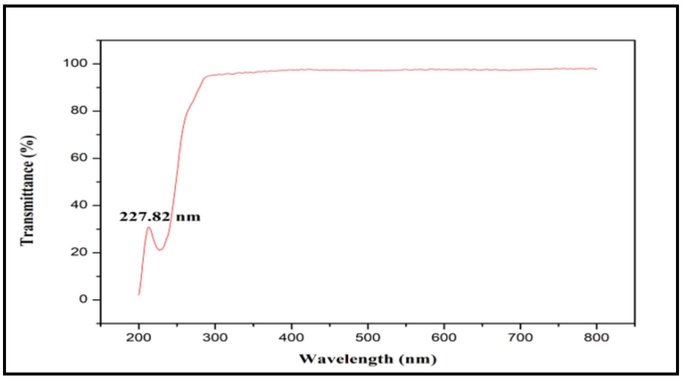

Fig. 4. UV Transmittance of LOMHA

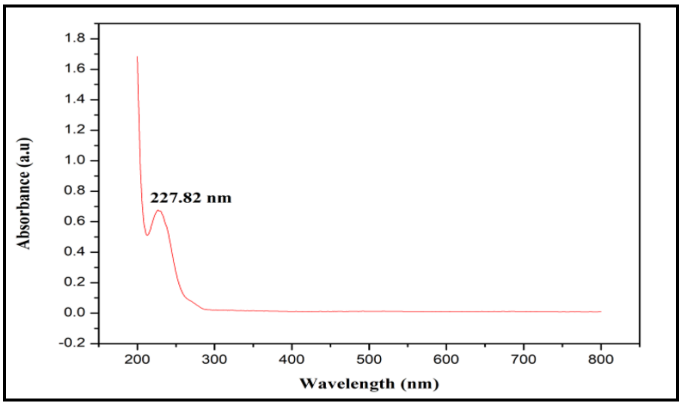

Fig. 5. UV Absorbance of LOMHA

The UV transmittance is used to found the cut off range of LMHA. The cut off range is 227.82 nm shown in Fig. 4. And the UV absorbance is used to found the cut off range of LMHA. The cut off range is 227.82 nm shown in Fig. 5.

3.5. Dielectric studies

In order to determine details of the electric field distribution, the dielectric response to frequency of the grown LOMHA crystal was examined. Fig.6. shows the measured dielectric constant change curves with applied frequency. The following relation can be used to determine the dielectric constant (ε) based on the measurement [12].

$$\varepsilon = Cd/\varepsilon_0 A$$

Here, ε is related to the capacitance of chosen crystal (C) with a thickness of 'd' and area of the chosen crystal 'A'. In LOMHA crystal, it is seen from the curves that the dielectric constant increases at lower frequency region which lowers at elevated frequencies. Such elevated dielectric constant can be associated with the polarization of electronic, ionic as well as dipolar and space charge in the LOMHA crystal. The Fig. 6. shows that the Log f dependent of Dielectric constant.

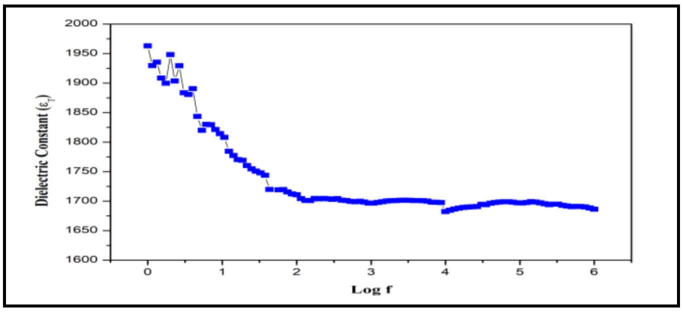

Fig. 6. Log f dependent of Dielectric Constant of LOMHA

At room temperature, dielectric loss with varying frequency was also measured which illustrated in Fig.7. The results demonstrate that the dielectric loss observed for the present crystal is lower at higher frequencies. The dielectric loss and dielectric constant suggest that the LOMHA crystal is suitable for NLO applications. Fig.7. shows that log f dependent of Dielectric Loss for LOMHA crystal.

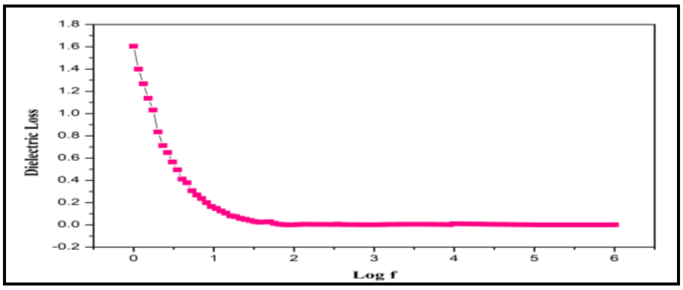

Fig. 7. Log f dependent of Dielectric loss of LOMHA

3.6. Thermo Gravimetric and Differential thermal Analysis

The phase transition, different stages of the decay of the crystal system and the water of crystallization of the crystal are given by the Differential thermo gram analysis (DTA) and Thermo gravimetric analysis (TGA) [13]. Thermal studies of LMHA crystal were analysed by

Thermo gravimetric Analysis (TGA) and Differential Thermal Analysis (DTA) between the room temperature and 700 °C in the PerkinElmer instrument at a rate of heating 25° C/min. The thermal image is shown in the Fig .(8). The material is found to be stable up to 250.64°C above the endothermic peak in DTA, which was identified at 250.64°C from the DTA curve [14].

After reaching an endothermic transition, the materials start to break down. The melting point in TG at which weight loss has been seen is determined to be the endothermic peak.

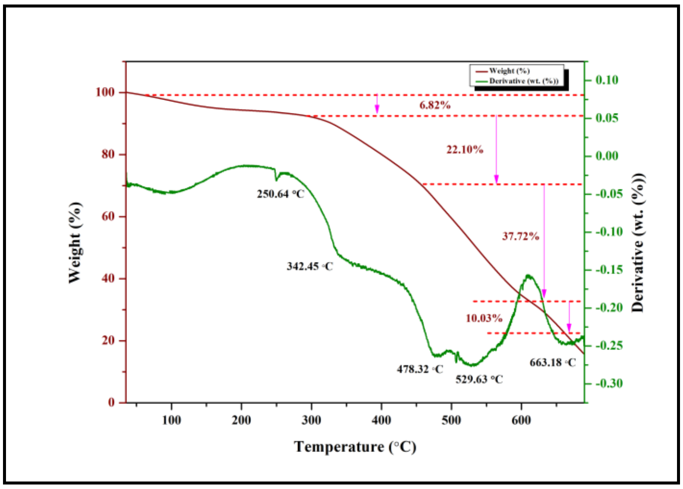

Fig. 7. Weight (%) vs Temperature (°C) vs Derivative(wt.(%)) DTA & TGA of LOMHA

3.7. Second harmonic generation efficiency

The NLO efficiency of LOMHA crystal was tested using Kurtz and Perry method. The sample was illuminated using Q-switched Nd: YAG laser with the first harmonic output of 1064 nm with a pulse width of 8 ns. The SHG was confirmed by the emission of green light (λ=532 nm). Thus the SHG efficiency of LOMHA is 1.2 times of KDP. Emission of green radiation from the sample confirms the presence of NLO property.

4. Conclusion

L-Ornithine Monohydrochloride doped Hippuric Acid Crystal is the new combination of Non-linear of optical organic crystal and it grown by the slow evaporation method. The powder XRD pattern of LOMHA crystal is plotted and its hkl values are matched. The FT-IR analysis the Hippuric acid doped L-Ornithine monohydrochloride crystal and found functional group and molecular structure. The UV-Visible analysis of absorbance and transmittance of the Hippuric acid doped L-Ornithine monohydrochloride crystal were analysed. The UV transmittance is used to found the cut-off range of LOMHA. The cut off range is 227.82 nm for both transmission and absorbance. The thermal characteristics of the crystal are investigated using the thermal gravimetric analysis. The material is found to be stable up to 250.64°C above the endothermic peak in DTA, which was identified at 250.64°C from the DTA curve. The dielectric constant and dielectric loss both were shows that the curves are increases at lower frequency region and indicates the LOMHA crystal is appropriate for NLO applications. LOMHA crystals have SHG efficiency 1.2 times greater than that of KDP.

Conflicts of Interest

The authors declare that they have no known conflicts of interests.

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