Available online at www.elixirpublishers.com (Elixir International Journal)

Crystal Research Technology

Elixir Crystal Research Tech. 68 (2014) 22296-22298

ISSN: 2229-712X

Synthesis, Growth, and Characterization of Nonlinear Optical Crystal: L-Alanine Lithium Nitrate

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ARTICLE INFO

Article history:

Received: 28 December 2013;

Received in revised form:

22 February 2014;

Accepted: 4 March 2014;

Keywords

UV-Vis Spectroscopy,

Powder X-ray diffraction,

FTIR Spectroscopy.

ABSTRACT

Nonlinear optical L-Alanine Lithium Nitrate (LALN) single crystal was grown by slow evaporation solution method at room temperature. The title compound was characterized by various methods such as UV-Vis Spectroscopy, powder X-ray diffraction and Fourier Transform infrared (FTIR) Spectroscopy. The grown LALN was found to crystallize in orthorhombic system with space group $P2_12_12_1$. The SHG efficiency of LALN was found to be 0.42 times that of potassium dihydrogen orthophosphate (KDP) and 0.12 times that of urea.

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Introduction

Nonlinear optical (NLO) crystals are vital for the development of laser science and technology, because only this kind of materials can change frequency of laser beam and modulate its amplitude and phase. The extensive research of suitable new nonlinear materials is an important task because of their application in telecommunication for efficient signal processing and optical information storage devices. Organic nonlinear optical materials are of current interest for they are being used in advanced optical data processing devices.[1,2]. Amino acids are good materials for NLO application because they contain proton donor carboxyl acids (-COO) group and the proton acceptor (NH_2) group [3,4]. Semi organic materials possess several attractive properties such as high NLO coefficient, high laser damage threshold and wide transparency range, high mechanical strength and thermal stability, which make the materials suitable for second harmonic generation (SHG) and other NLO applications. A series of studies on semiorganic amino acid compounds such as L-arginine phosphate (LAP),[5] L-arginine hydrobromide (L-AHBr),[6] L-histidine tetrafluoroborate (L-HFB),[7] L-arginine hydrochloride (L-AHCl),[8] L-alanine acetate (L-AA),[9] and glycine sodium nitrate (GSN)[10] as potential NLO crystals have been reported. In this paper, we report the growth of L-alanine Lithium Nitrate (LALN) by SEST method.

Experimental:

Synthesis and crystal growth:

LALN was synthesized from aqueous solution of L-Alanine and Lithium Nitrate (AR grade) taken in the equimolar ratio. In solution growth technique, the solubility of material in the solvent plays a vital role in growing large-size single crystal. In order to select the proper solvent for growing large-size single crystals, the solubility of LALN in various solvents were studied. The solubility of LALN in organic solvents like acetone, ethanol, and methanol was found to be very less. Water was found to be a better solvent because of the low evaporation rate compared to other organic solvents. The calculated amount of the reactants were thoroughly dissolved in double distilled water and stirred well for about 2 hours using a magnetic stirrer to obtain a homogeneous mixture.

The completely dissolved solution was filtered using filter paper to remove the suspended impurities and then allowed to crystallize by slow evaporation of solvent at 30˚C. The crystallization took place in 22 days and high quality transparent crystals of size 2×0.5×1 mm^3 were harvested.

Characterization:

The UV-Vis transmittance spectrum was recorded using a Shimadzu UV-1061 UV –visible spectrometer. The single crystal X-ray diffraction (XRD) analysis of LALN crystal was carried out using a MESSRS ENRAF NONIUS X-ray Diffractometer and its unit cell dimensions were determined. The crystalline quality was found by PAN Analytical Power XRD. Fourier Trans- form infrared (FTIR) spectrum was recorded by the KBr Pellet technique using SHIMADZU Spectrometer for the range 400–4000cm^{-1} to confirm the functional groups. The NLO behavior of L-alanine lithium nitrate crystal was tested by Kurtz powder SHG test using Nd:YAG laser (1064 nm).

UV-Visible Spectral analysis

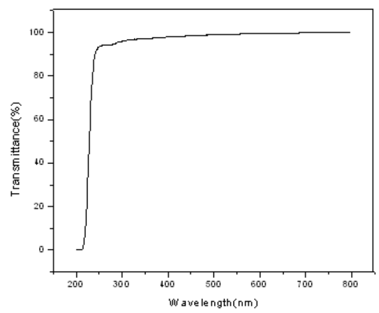

Figure 2. UV-Vis spectra for LALN

Transmission spectral studies are very important for any NLO material must have wide transparency window for optical applications. The UV-Vis transmittance spectrum for the wavelength range between 200nm and 900 nm was recorded using a Shimadzu UV-1061 UV –visible spectrometer. The UV-Vis transmittance spectrum is shown in figure2 for LALN single

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crystal. The UV cutoff wavelength was around 250nm. This is an advantage of the use of amino acids where the absence of strongly conjugated bonds leads to wider transparency ranges in the visible and UV spectral regions [11].There is no absorption of light in the visible range of the electromagnetic spectrum, and it can be used as a potential material for SHG or other applications in the blue and violet regions.

X-ray diffraction studies:

The fine power of the title compound has been subjected to powder X-ray diffraction analysis and the recorded pattern is shown in figure [3]. The powder sample was scanned in steps of 1° for a time interval of 10 seconds over a 2ϴ range of 10° to 70°. The sharp and well defined Bragg's peaks at specified 2ϴ angles show the crystalline nature and purity of the crystal. New peaks in the XRD pattern of the grown crystal confirm the incorporation of lithium nitrate in the grown crystals.

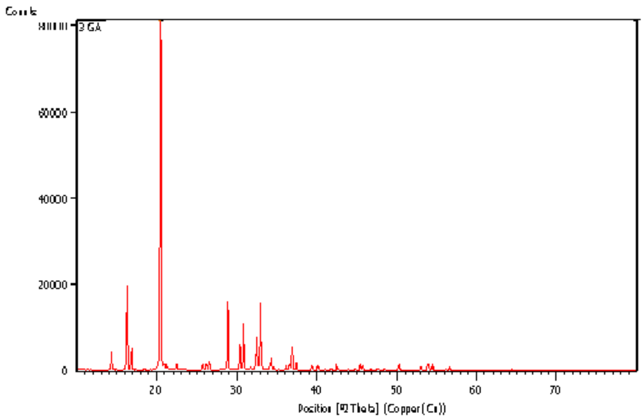

Figure 3. Powder X-ray diffraction pattern for LALN

The grown LALN crystal has been investigated by single crystal XRD and lattice parameters obtained are a= 5.775A˚, b= 6.020A˚, and c= 12.316 A˚, & α = β = γ =90° and the cell volume =428.1A˚. The structure is confirmed to be orthorhombic with the space group $P2_12_12_1$.

Fourier Transform Infrared (FTIR) analysis

The infrared spectrum of the grown crystal has been taken in the range of 400-4000cm^{-1}. The Fourier transform infrared (FTIR) spectrum of LALN is shown in figure 4.The presence of the functional groups in LALN crystal are identified. The sharp absorption peak at 2110.12 cm^{-1} is due to combination of NH_3^+ symmetric stretching and torsional oscillation. The prominent absorption band is relatively strong due to symmetric NH_3^+ bending at 1508 cm^{-1}. The peak at 1411 cm^{-1} that is assigned to the COO^- symmetric stretching and COO^- bending vibration at 1377 cm^{-1} were identified. The peaks are attributed to the rocking deformation of NH_3^+ group at 1149 cm^{-1} and 1111 cm^{-1}. The peak 918 cm^{-1} is due to C-C-N symmetric stretching. The rocking vibrations of COO^- are observed at 536 cm^{-1} and 486 cm^{-1} respectively.

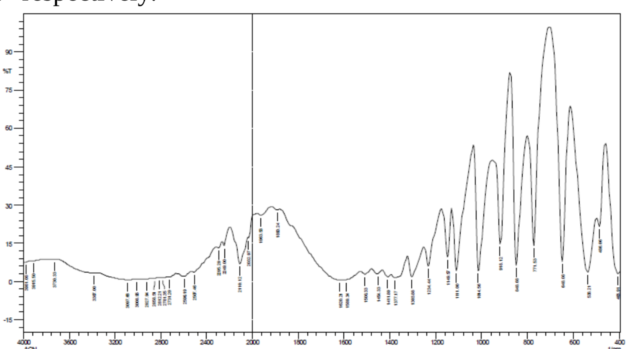

Figure 4. FTIR Analysis for LALN

Table 1. FTIR Assignment of LALN crystal

LALN crystal	Assignment
3097	NH_3^+ asymmetric stretching
2596	NH_3^+ stretching vibration
2249	Stretching of CH_3 vibration
2110	Combination of symmetric NH_3^+ bending vibration & torsional oscillation
1508	NH_3^+ symmetric bending
1454	CH_3 bending
1411	COO^- symmetric stretching
1377	COO^- bending vibration
1303	CH_2 wagging
1234	CH_3 stretching
1149	rocking deformation of NH_3^+
1111	rocking deformation of NH_3^+
1014	CH_3 rocking
918	C-C-N symmetric stretching
848	C-H bending
771	CH_2 rocking
648	O-C= O in plane deformation
536	COO^- rocking
486	COO^- rocking

Second harmonic generation (SHG) studies

The second harmonic generation behavior of the powdered material was tested using the Kurtz and Perry method [12]. A high intensity Nd:YAG laser (λ = 1064 nm) with a pulse duration of 6 ns was passed through the powdered sample. The SHG behaviour was confirmed from the output of the laser beam having the green emission (λ = 532 nm). It is a potential material for frequency conversion. The second harmonic generation signal of 4.9 mV for LALN crystal was obtained for an input energy of 3.6Milii Joules/Pulse. But the standard KDP crystal gave an SHG signal of 11.6mVfor the same input energy. Thus, it is observed that the SHG efficiency of the grown LALN single crystal is 0.42 times that of the standard KDP crystal.

Conclusion

Nonlinear optical LALN single crystal has been grown by slow evaporation method at room temperature. The sharp and well defined Bragg's peaks of powder XRD pattern at specified 2ϴ angles shows the crystalline nature and purity of the crystal. The lattice parameters of LALN are determined by single crystal XRD. It belongs to orthorhombic crystal system with the space group $P2_12_12_1$.Grown crystals were subjected to FTIR analysis, to confirm the presence of various functional groups in LALN single crystals. The lower cutoff wavelength at 250nm and the wide transparency range (200nm–900nm) was observed from the UV–Vis spectrum confirms its suitability of the material for SHG applications. The NLO property of the grown crystal was also studied by Kurtz–Perry SHG test.

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