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Synthesis, growth and characterization of non-linear optical material: L-Tryptophan p-nitrophenol (LTPNP) single crystal

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ABSTRACT

A new nonlinear optical organic crystal L-tryptophan p-nitrophenol (LTPNP) of dimension 19 mm × 2 mm × 1.5 mm has been grown from an aqueous solution for the first time by slow evaporation technique at ambient temperature. The crystal structure of LTPNP was confirmed by single crystal X-ray diffraction. LTPNP crystallizes in non-centrosymmetric monoclinic system with space group P_{21}. The recorded FTIR spectrum confirms the presence of various functional groups in the grown crystal and confirms the formation of LTPNP. Thermal stability and melting temperature of the LTPNP crystal were identified from TG/DTA analysis. The optical absorption study confirms the suitability of the crystal for device applications. LTPNP exhibits SHG efficiency over 1.7 orders of magnitude higher than that of urea and 4 orders of magnitude higher than that of KDP.

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1. Introduction

Nonlinear optical materials (NLO) have proven to be an interesting candidate for a number of applications such as second harmonic generation, frequency mixing, electro-optic modulation, etc. In recent years, organic NLO materials are attracting a great deal of attention for possible use in optical devices because of their large optical nonlinearity, low cut-off wavelengths, short response time and high laser damage thresholds [1]. Considerable work has been done in order to understand the microscopic origin of nonlinear behavior of organic materials [2–5]. To possess NLO property, organic materials should contain highly conjugated π-electron system affected by electron donor and acceptor groups. The NLO properties of large organic molecules and polymers have been the subject of extensive theoretical and experimental investigations during the past two decades and they have been investigated widely due to their high nonlinear optical properties, rapid response in electrooptic effect and large second or third order hyperpolarizabilities compared to inorganic NLO materials [6]. Thus, there is much impetus to design and understand organic compounds for SHG applications.

Nowadays complexes of amino acids have also been proved as attractive materials in optical applications, as they contain a proton donating carboxyl group and proton accepting amino group [7]. In this paper, we have reported the synthesis, growth and characterization of L-tryptophan p-nitrophenol. It is an organic crystal with excellent nonlinear coefficient. The structure of L-tryptophan p-nitrophenol trisolvate crystal grown using hot methanol as solvent was reported by Rodrigues et al. [8]. Compared with Rodrigues et al. work, we have grown the crystals using water as a solvent for the first time instead of alcoholic solvents. The crystal structure was determined by X-ray diffraction studies and was found to be monoclinic. In the present investigation we report the optical, thermal and second harmonic generation properties of LTPNP.

2. Growth of LTPNP single crystals

The low temperature solution growth technique is used for the growth of LTPNP which has been widely used for the growth of organic and inorganic single crystals to get more transparent single crystals. The starting compounds, namely, L-tryptophan (Loba Chemie, 99%) and p-nitrophenol (Alfa Aesar, 95%) were used without further purification. The single crystals of LTPNP have been successfully grown from slow evaporation solution growth technique at room temperature in the stoichiometric ratio, 1:1 with deionized water as solvent. The saturated solution of LTPNP was obtained by dissolving the charge material into the deionized water with continuous stirring of the solution using an immersible magnetic stirrer at room temperature for about 4 h and the solution was optimally closed for controlled evaporation. The repeated recrystallization was carried out to improve the purity of the grown crystal, which in turn enhances the optical quality of the growing

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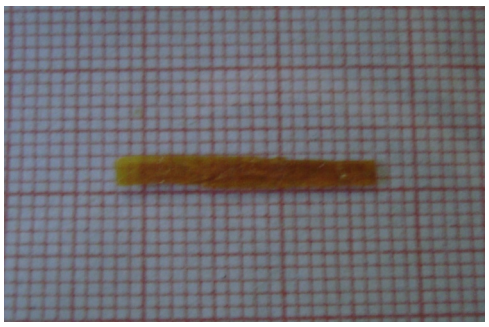

Fig. 1. Grown single crystal of LTPNP.

crystals. Single crystals of typical size 19 mm × 2 mm × 1.5 mm were obtained from the mother solution after 10 days (Fig. 1).

3. Results and discussion

3.1. Single crystal X-ray diffraction analysis

The single crystal X-ray diffraction analysis of the grown crystal was carried out using Bruker Nonius APEX II – V2.D2 single crystal diffractometer with Mo Kα (λ = 0.717 Å) radiation. From the single crystal XRD analysis it is observed that the grown crystal belongs to monoclinic system with space group P_{21}. The lattice parameter values are presented in Table 1 which is in good conformity with the published values [8].

3.2. Powder X-ray diffraction analysis

Finely crushed powder of the grown LTPNP crystal was subjected to powder X-ray diffraction analysis using Cu Kα (40 kV, 30 mA) radiation. The sample was scanned over the range 4–90° at a scan rate of 2°/min. The recorded X-ray diffraction pattern of LTPNP is shown in Fig. 2. Using the simulated (*hkl*) values and the experimental *d* values, the lattice parameters were estimated by TJB Holland & SAT Redfern unit cell software package and the calculated lattice parameter was found to be in close agreement with the single crystal X-ray diffraction data.

3.3. Density measurements

The density of the LTPNP crystal was determined as 1.401 g/cc by the floatation method using a liquid mixture of CCl_4 and bromoform. The expected density (ρ) of the LTPNP was calculated from the crystallographic data, using the well-known expression [9].

$$\rho = \frac{MZ}{N_A abc} \quad (\mathrm{g/cm^3})$$

where *M* is molecular weight of LTPNP; molecular unit cell *Z* = 2; N_A is Avogadro's number and *a*, *b* and *c* are the lattice parameters of LTPNP crystal. The experimentally measured density is in good agreement with the theoretical values.

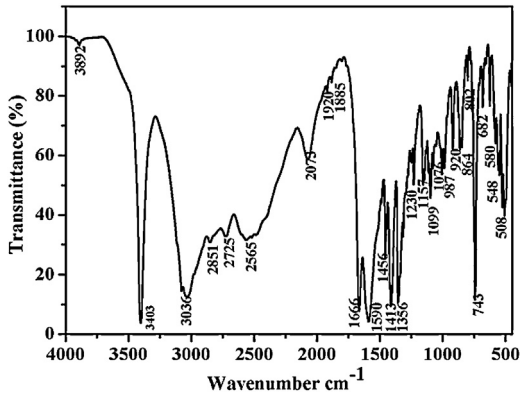

Fig. 3. FTIR spectrum of L-tryptophan.

3.4. FTIR spectral analysis

The functional groups of LTPNP crystals were analyzed by FTIR spectroscopy which was recorded by Shimadzu IR Affinity 1 spectrometer in the wave number range 400–4000 cm^{-1} at room temperature using KBr pellet technique. The recorded FTIR spectrum for L-tryptophan, p-nitrophenol and LTPNP are shown in (Figs. 3–5) for comparison. In the high frequency region sharp intense peaks at 3437 cm^{-1} and 3205 cm^{-1} are attributed to asymmetric stretching vibrations of NH and NH_3^+. The peak obtained at 2816 cm^{-1} was due to symmetric C—H stretching of the amino acid. The peaks obtained at 1635 cm^{-1} and 1408 cm^{-1} were due to asymmetric and symmetric stretching vibrations of COO^- of carboxyl group. The presence of nitro group was confirmed by the peaks at 1492 cm^{-1} and 1327 cm^{-1}. The peaks at 744 cm^{-1} and 690 cm^{-1} indicate the C—H bending [10] (Table 2). The above assigned peaks of various functional groups confirm the formation of LTPNP.

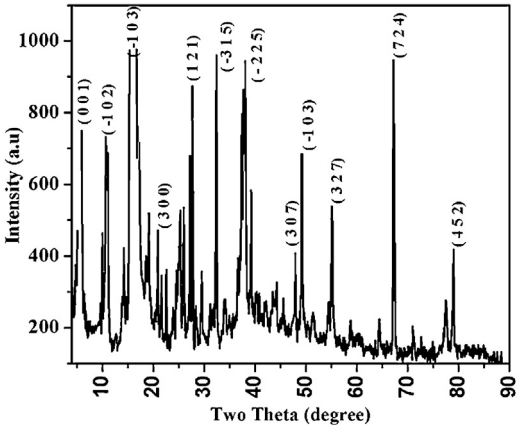

Fig. 2. Powder XRD pattern of LTPNP crystal.

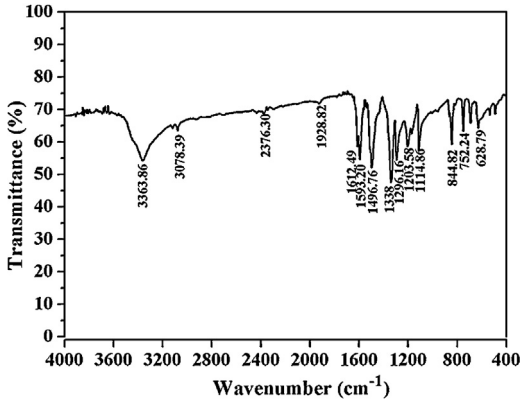

Fig. 4. FTIR spectrum of p-nitrophenol.

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