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Study on growth, spectral, optical and thermal characterization of an NLO crystal: 6-Methyl nicotinic acid (6MNA)

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ABSTRACT

6-methyl-nictinic acid (6MNA), organic non linear optical (NLO) single crystals were grown by slow evaporation solution technique. The cell parameters of 6MNA were confirmed from single crystal X-ray diffraction analysis. The Fourier transforms infrared and proton Nuclear magnetic resonance spectral analysis confirm the presence of various functional groups and the placement of protons respectively in 6MNA compound. UV–vis–NIR spectral studies revealed that the grown 6MNA has good optical transmission in the range of entire visible region. The thermal properties of crystals were evaluated from thermogravimetric (TG) and differential thermal analysis (DTA). It has shown that the grown crystals were stable up to 213°C. The second harmonic generation (SHG) measurements indicated that the efficiency of 6MNA is two times greater than that of the KDP crystals and is suitable for frequency conversion applications.

1. Introduction

In the recent year, the nonlinear optical crystals, both organic and inorganic, with large second-order optical nonlinearities, attracted the materials scientists. These materials have a significant impact on optical communication, remote switching, laser technology and optical storage technology etc. In the few decades, many organic and inorganic materials have been developed to cover the possible applications in ultra-violet, near and far- infrared wavelength regions [1–3]. Great attention has been paid to organic NLO materials due to their promising applications in optoelectronics and the much larger non-linear response, very fast switching time and convenient optimization routs through molecular engineering compared to the currently studied inorganic materials [4–6]. Many organic compounds show good NLO property due to the presence of π-bonds, which helps in the molecular engineering for the tailor made applications. With cascaded frequency conversions, deep UV coherent light can be produced in solid state lasers using NLO crystals. Large second order NLO response is possible in the molecule with various delocalization π electrons, since there will be a change in the dipole moment from ground state to keyed up state which will have large transition moment and noncentro symmetric response [7–9].

Recently, several investigations have been carried out on the complexes of pyridine carboxylic acids, namely nicotinic, isonicotinic acid and picolinic acids. This has led to their use in various fields including electronics; for instance, in electroluminescent devices in analytic tools, functional biological assays and in medical imaging devices [10–12]. Single crystals are the backbone of the modern technological revolution. The impact of single crystals is clearly visible in industries that deal with semiconductors, laser technology etc. Most of the high performance.

Optoelectronic devices are made from crystalline materials [13,14]. We report the results of our work on 6-methyl nicotinic acid (6MNA) single crystals right from the crystal growth by slow evaporation solution growth and various characterizations such as singly crystal XRD, spectral, optical, and thermal and powder SHG measurements.

2. Materials and methods

2.1. Crystal growth

The commercially available 6-methyl- nictinic acid (6MNA) (AR grade) was purified by repeated crystallization process before growth as it would improve the purity of the material, which in turn would enhance the optical quality of the crystals. As the growth process and the quality of the crystals significantly depend on super saturation, the

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