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Investigation about nonlinear optics and antibacterial activity of pyrrolidine-2-carboxylic acid cadmium chloride hydrate single crystal

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ABSTRACT

This work intends to investigate the superior properties of Pyrrolidine-2-carboxylic acid Cadmium Chloride Hydrate (PCCH) that was grown by the slow evaporation technique at room temperature. The crystalline nature of PCCH was found by powder X-ray diffraction analysis. The optical behaviour of the grown crystal was unveiled by using UV-vis-NIR. The refractive index of the crystal was measured experimentally using Metricon prism coupler for the first time. The z-scan measurement was taken to explore the third harmonic generation efficiency of the grown crystal for the first time. The structural imperfections were analyzed by performing the etching studies on the grown crystal. The first attempt of antibacterial activity of this crystal was carried at different concentrations (25, 50, 75 and 100 μg/mL) in-vitro against *Staphylococcus epidermis* (G + Ve); *Escherichia coli, Vibrio cholera* (G–Ve) bacteria. These studies established that PCCH crystals might find useful applications in the field of biomedical and nonlinear optics.

1. Introduction

The natural aminoacids are of organic materials exists in dipolar nature (NH_3^+ and COO^-) and exhibit the nonlinear optical properties arising from the intramolecular charge transfer between two groups of opposite nature [1]. Pyrrolidine-2-carboxylic acid is a α-imino acid which contain both imino (-NH) and carboxyl (-COOH) functional groups, differing in the bonding to the nitrogen from amino acids and it is widely used as a laser frequency doubler and electro optic modulator. It is unique among other aminoacid, which contains a pyrrolidine ring in the side chain that makes it rigid and directional in biological systems [2]. The hydrogen bond of CH—O molecule in Pyrrolidine-2-carboxylic acid plays an important role in the formation of supermolecule and perhaps involve in the generation of noncentrosymmetric structure [3,4]. It has formed several complexes, which are promising materials for NLO applications exhibiting excellent physical and chemical properties [5,6]. The structure of PCCH was solved in 1983 by Yasuhiko Yukawa et al. [7]. In the present study, single crystal of Pyrrolidine-2-carboxylic acid cadmium chloride hydrate was grown and their structural, linear, nonlinear, refractive index, etching and antibacterial activity are discussed in the application point of view. This material is a promising one for biomedical applications, laser technology and optical data storage as they tend to exhibit excellent antibacterial activity and third harmonic generation.

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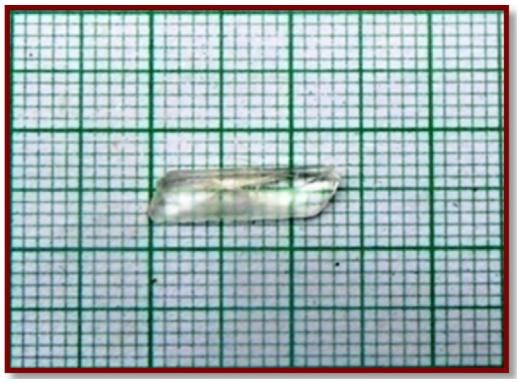

Fig. 1. Photograph of as grown crystal of PCCH.

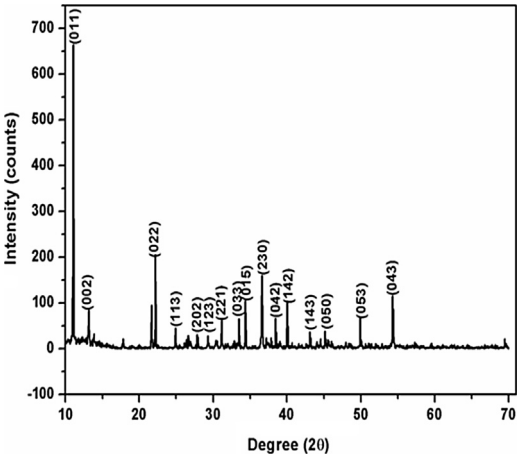

Fig. 2. Powder XRD pattern of PCCH.

2. Experimental

2.1. Synthesis and crystal growth

AR grade materials of Pyrrolidine-2-carboxylic acid and cadmium chloride hydrate were taken in the equimolar ratio as given in Eq. (1) and dissolved in the solvent of deionized water under constant stirring for 2 h at room temperature. The resultant solution was filtered and allowed to evaporate at room temperature. Optically good quality crystals of PCCH were harvested in a time span of 15 days. The purity of the crystal was improved by the successive recrystallization process followed by slow evaporation which yields well defined crystals up to the size of $14 \times 5 \times 2\,mm^3$ as shown in Fig. 1.

$$C_5H_9NO_2 + CdCl_2{\cdot}H_2O\,CdCl_2{\cdot}H_2O \rightarrow Cd(C_5H_9NO_2)Cl_2{\cdot}H_2O \quad (1)$$

Pyrrolidine-2-carboxylic acid cadmium chloride hydrate PCCH

3. Characterization

3.1. X-ray diffraction analysis

The cell dimension was obtained in the earlier report from single crystal X-ray diffraction studies which reveals the orthorhombic structure of PCCH with the space group of C2 [8,9]. The crystalline structure of the PCCH crystal was characterized by using powder XRD using PHILIPS 'X'Pert Pro Radiation CuKα X-ray diffractometer in the range of 10–70° with a scan speed of 1°/min and the diffraction peaks were indexed by using "powder X" software as shown in Fig. 2. The sharp and intense peaks in the pattern affirm the high crystallanity and goodness in quality of the PCCH crystal [10]. The obtained diffraction peaks in the pattern are matched with the reported values [8,11].