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Studies on the growth, spectral, structural, electrical, optical and mechanical properties of Uronium 3-carboxy-4-hydroxybenzenesulfonate single crystal for third-order nonlinear optical applications

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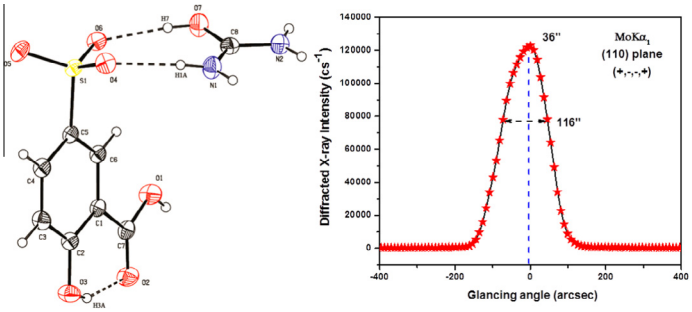
HIGHLIGHTS

- Single crystal of UCHBS size up to $16 \times 12 \times 4$ mm^3 was grown by solution growth method.
- FWHM traced on (1 1 0) plane of UCHBS crystal was found to be 116 arc s.
- UV–Vis cut-off wavelength of UCHBS was found to be 345 nm.
- NLO parameters, $n_2 = 3.932 \times 10^{-12}$ m^2/W, and $\beta = 2.653 \times 10^{-4}$ cm/W were estimated.

GRAPHICAL ABSTRACT



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ABSTRACT

Organic Uronium 3-carboxy-4-hydroxybenzenesulfonate (UCHBS) nonlinear optical single crystal was grown by solution growth technique. The solubility and nucleation studies were performed for UCHBS at different temperatures 30, 35, 40, 45, 50 and 55 °C. The crystal structure of UCHBS was elucidated from single crystal X-ray diffraction study. High resolution X-ray diffraction technique was employed to study the perfection and internal defects of UCHBS crystal. Infrared and Raman spectra were recorded to analyze the vibrational behavior of chemical bonds and its functional groups. The physico-chemical changes, stability and decomposition stages of the UCHBS compound were established by TG–DTA studies. The dielectric phenomenon of UCHBS crystal was studied at different temperatures with respect to frequency. Linear optical properties of transmittance, cut-off wavelength, band gap of UCHBS were found from UV–visible spectral studies. Third-order nonlinear optical susceptibility, nonlinear refractive index, nonlinear optical absorption coefficient values were measured by Z-scan technique. The mechanical properties of UCHBS crystal was studied by using Vicker's microhardness test. The growth features of UCHBS crystal were analyzed from etching studies.

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Introduction

Recently, materials with excellent nonlinear optical (NLO) properties and fast response have attracted much attention for their widespread applications in optical switching, signal processing, optical power limiting and optical communications, optical data storage applications [1–3]. Due to these challenging applications, the growth of optical single crystals is very important for the fabrication of technologically important devices [4–6]. The use of single crystals is clearly noticeable in electronics and optics [7]. The high NLO property is the needed quality for advanced hybrid materials useful in next generation optical technologies. It was found that organic materials show excellent nonlinearity than inorganics. The delocalized π-electron system enhances their asymmetric polarizability and it leads to the microscopic origin of nonlinearity in molecular organic NLO materials [8]. The novel molecular designs with higher third-order nonlinearity and to incorporate them into the devices are the urgent need for optical applications [9,10]. Urea based compounds offered a wide choice of materials and expected to play an important role in future [11]. The acid component 5-Sulfosalicylic acid is an excellent hydrogen donor and hydrogen acceptor and used to design novel crystal with Urea. 5-Sulfosalicylic acid has three potential coordination sites and it can give mono-, di- and tri-anionic ligand species through deprotonation. The presence of large amount of oxygen atoms in the functional groups can be afforded hydrogen bonded associations and used to self-assembly of crystallization [12]. In the present report, Uronium 3-carboxy-4-hydroxybenzenesulfonate (UCHBS) crystal was grown from aqueous solution by slow evaporation method. The grown UCHBS crystals were subjected to X-ray diffraction, infrared, Raman, thermal, dielectric, UV–visible spectral studies and mechanical studies. The third order nonlinear optical property of UCHBS crystal studied by employing Z-scan technique and results are presented.

Materials and methods

The analytical grade starting materials Urea and 5-Sulfosalicylic acid were used for synthesis of UCHBS compound. BRUKER KAPPA APEX II X-ray diffractometer was used to determine the crystal system and lattice parameters of UCHBS crystal at 293 K. High resolution X-ray diffraction curve was recorded by using PANalytical X'PertPRO MRD system with MoK$_{\alpha 1}$ radiation to assess the crystalline perfection. BRUKER IFS FT-IR and Bruker RFS27 spectrophotometers with 100 mW laser excitation were used to record Infrared (IR) and Raman spectrum respectively. TGA–DTA thermogram was traced from RT to 600 °C using SDT Q600 V8 instrument. The dielectric measurements were carried out by using HIOKI 3532-50 LCR HITESTER in the frequency range 50 Hz–5 MHz. UV–visible spectrum was recorded for the grown crystal using VARIAN CARRY 5E photospectrometer. Z-scan technique was employed to determine third-order nonlinearity using He–Ne laser source at 632.8 nm. Vicker's microhardness test was carried out for UCHBS crystal using Shimadzu HMV-2000 Vicker's pyramidal indenter.

Experimental

Synthesis, solubility, metastable zone width and crystal growth

Uronium 3-carboxy-4-hydroxybenzenesulfonate (UCHBS) compound was synthesized by dissolving equimolar quantity of Urea (6.006 g) and 5-Sulfosalicylic acid (25.422 g) in 100 ml deionized water and stirred. The solution was magnetically stirred about 8 h to achieve homogeneous mixture and synthesized (Fig. 1). It was dried at room temperature and synthesized salt was collected. Repeated recrystallization process was adopted for purification of UCHBS salt in aqueous solution and impurities were removed by filtration.

The solubility and metastable zone width measurements were carried out in a constant temperature bath with an accuracy ± 0.01 °C. The solubility was determined by gravimetric analysis at different temperatures ranging 30–55 °C. 100 ml of deionized water (solvent) was taken in a flask and UCHBS salt was added up to the saturation point at 30 °C. The solution was stirred for about 8 h to achieve homogenization by using an immersible magnetic stirrer and saturated solution was achieved. 10 ml of saturated solution was taken out and poured into the petri dish and dried. Then, the dried UCHBS salt was weighed. The same process was repeated for other temperatures. The solubility of UCHBS is shown in Fig. 2. From the plot, it was observed that solubility curve shows a positive gradient which is suitable for slow cooling and evaporation crystal

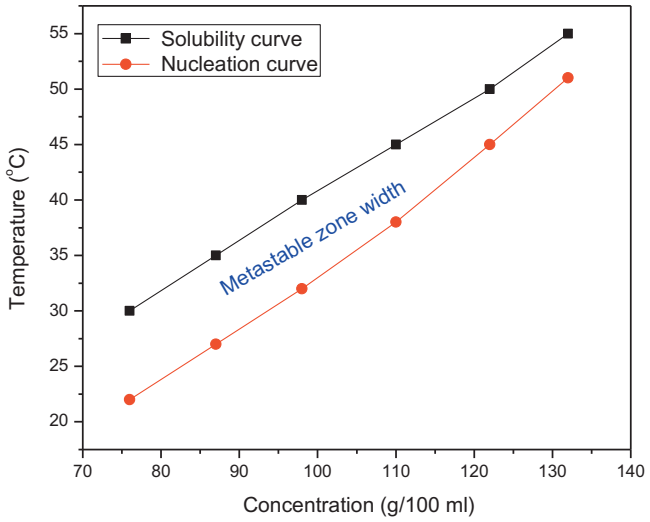

Fig. 2. Solubility and nucleation curves of UCHBS in water solvent.

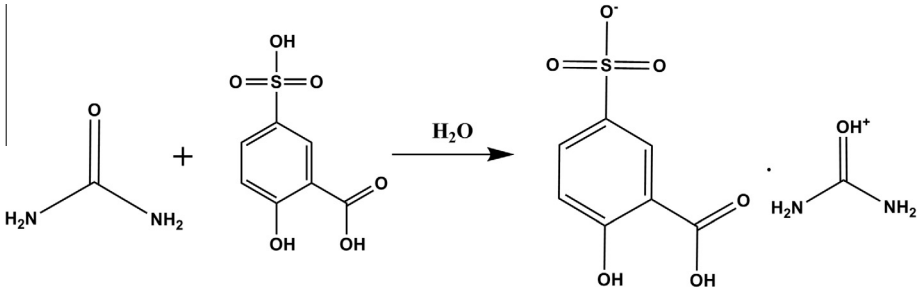

Fig. 1. Material synthesis scheme for UCHBS.