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Creatininium 4-nitrobenzoate – A phase matchable organic nonlinear optical material with large laser-induced damage threshold value for optoelectronics applications

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ABSTRACT

A promising organic nonlinear optical (NLO) material of creatininium 4-nitrobenzoate (C4NB) was grown as single crystals using slow evaporation solution technique. The grown crystal was crystallized in orthorhombic system of acentric space group, $P2_12_12_1$. The crystalline nature was analyzed by powder X-ray diffraction study. The molecular structure was evidently established by using ^{1}H and ^{13}C NMR spectral analysis. The UV-vis-NIR spectrum showed high optical transparency of C4NB crystal in Vis-NIR region with lower cut-off wavelength at 353 nm. Thermal analysis revealed that C4NB crystal was thermally stable up to 225 °C. The dielectric behavior was studied at different temperatures as a function of frequency varies from 50 Hz to 5 MHz. The mechanical nature and photoconductivity behaviour were carried out effectively for grown crystal. The NLO phase matching and laser-induced damage threshold (LDT) characteristics of C4NB crystal was done by Nd:YAG laser and compared with other organic crystals. All these characterizations and their results recognized that grown crystal may be exploited for optoelectronics applications in near future.

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1. Introduction

NLO materials are predominant research interest of material scientist's owing to its crucial functions of frequency conversion and mixing, electro-optical modulation, optical switching, parametric amplification, optical bistability and laser remote sensing in the vast area of telecommunication, signal processing, quantum electronics and laser field such as medical and spectroscopic research [1–3]. So, enormous research efforts have been taken recently on the development of NLO materials to satisfy all these necessary characteristics. Organic materials are relatively exhibiting strong NLO response owing to the presence of delocalized electrons at π-π* orbitals [4–6]. Moreover, organic materials are the best supplant for the custom made inorganic materials used in frequency doubling, switching and modulation applications due to its wide range of key advantages including intrinsic nonlinearity, designing and synthetic flexibility for tailoring desired properties towards certain applications. These crucial characteristics exploited extensive search for an efficient NLO materials among organic materials. The promising NLO materials are expected to have the following essential properties for application perspectives such as high optical transparency, low dielectric constant, low refractive index, large damage threshold (LDT) and easier in crystal growth and device fabrication. So, the aim is to discover and develop an organic NLO material and simultaneously satisfy all the technological necessities mentioned earlier. This communication describes the synthesis, growth and some essential characteristics related to the practical applications of an organic NLO material. Creatinine is a superlative proton acceptor and 4-nitrobenzoic acid is an excellent proton donor involved in formation of many organic proton transfer complexes individually. Recently, guanidinium 4-nitrobenzoate [7], L-arginine p-nitrobenzoate monohydrate [8], L-histidinium 4-nitrobenzoate [9], 2-amino-4-methylpyridinium 4-nitrobenzoate [10] and 2-amino-6-methylpyridinium 4-nitrobenzoate [11] organic NLO single crystals have been grown successfully using 4-nitrobenzoic acid and exhibited optimal SHG efficiency with admirable properties. Similarly, creatininium succinate an efficient organic NLO material was reported with some promising characteristics including high thermal stability up to 247 °C, low dielectric constant (ε_r = 8.5) and large laser induced damage threshold value up to 5.2 GW/cm^2 [12]. In this work, a promising organic NLO material, creatininium 4-nitrobenzoate ($C_{11}H_{12}N_4O_5$) single crystals were grown

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and characterized well for identifying its utility for real-world applications. In this material, creatininium ($C_4H_8N_3O^+$) cation comprised an electron donor (NH_2) group and 4-nitrobenzoate ($C_4H_4NO_4^-$) anion contained an electron acceptor (NO_2) group which involved in intramolecular charge transfer (ICT) process causes enhanced optical nonlinearity [13]. The X-ray diffraction, spectral (^{1}H and ^{13}C NMR and UV-vis-NIR), thermal (TG-DTA and DSC), dielectric, photoconductivity, Vickers microhardness and laser (phase matching and LDT) studies were carried out for grown C4NB crystals and their results were discussed.

2. Material synthesis and crystal growth

The AR grade, creatinine (0.45 g, 0.4 M) and 4-nitrobenzoic acid (0.67 g, 0.4 M) compounds were dissolved in 30 ml of double distilled water in an equimolar ratio. The homogeneous solution was obtained by constant stirring for 90 min with hot plate environment at 40 °C. The prepared solution was filtered and covered by good quality tiny holed polythene paper to control past evaporation of the solvent and to maintain dust free environment. After slow evaporation of 9 days, crystalline substances of C4NB were obtained. The chemical scheme of C4NB is illustrated in Fig. 1a. The purity of the title compound was enhanced by consecutive recrystallization process. PXRD study was carried out for the C4NB crystal to evaluate its purity. The saturated solution was prepared from the obtained product using distilled water as a solvent. After slow evaporation of 6 days, optically good quality pale yellow color single crystals of C4NB were harvested from the solution and their photographs are shown in Fig. 1b. The density of the grown C4NB crystal was measured as 1.48 Mg m^{-3} using floatation method [14]. The liquid mixture of carbon tetrachloride (1.59 Mg m^{-3}) and xylene (0.89 Mg m^{-3}) were used for this measurement. The measured density value was found to be different from the parent compounds creatinine (1.09 Mg m^{-3}) and 4-nitrobenzoic acid (1.58 Mg m^{-3}), which confirmed the C4NB complex formation.

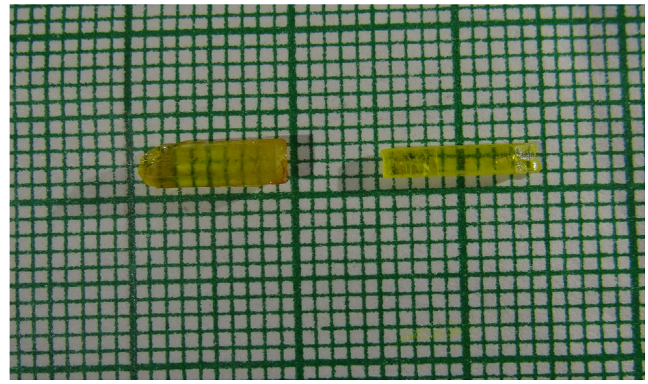

Fig. 1b. Photograph of as grown C4NB crystal.

3. Characterization techniques

In order to establish the chemical structure of grown C4NB crystal, ^{1}H and ^{13}C NMR spectra were recorded using a Bruker 500 MHz spectrometer in deuterated DMSO solvent. The nickel filtered, Cu Kα (λ = 1.5418 Å) radiation of X-rays equipped PANalytical XPERT-PRO powder X-ray diffractometer were used for powder X-ray diffraction measurement. Varian, Cary 5000 model spectrophotometer was employed to record UV-vis-NIR transmission spectrum in the range of 200–2200 nm. Simultaneous Thermal Analyzer SDT Q600 V8.3 was employed to perform thermogravimetric and differential thermal analysis in the temperature range between 50 and 950 °C at a heating rate of 20 °C/ min in a nitrogen atmosphere. Perkin Elmer DSC-4000 model differential scanning calorimeter was employed to record DSC curve in the temperature range between 50 and 500 °C at a heating rate of 20 °C. Hioki LCR 3532-50 LCR meter was used for dielectric measurement at different temperature in the frequency range of 50 Hz–5 MHz. Keithley 6517B electrometer was employed for photoconductivity measurement. Shimadzu HMV-2000 series Vickers Microhardness using pyramidal indenter was utilized for mechanical analysis.

4. Results and discussion

4.1. ^{1}H and ^{13}C NMR spectral studies

The crystallized compound was characterized by ^{1}H and ^{13}C NMR spectroscopy and recorded spectrum were shown in Figs. 2a and 2b. The ^{1}H NMR (Fig. 2a) clearly showed that C4NB compound contained 4 set of proton signals (NH_2 may not appear). The appearance of two doublets at δ 8.15 ppm and δ 8.29 ppm for four protons confirmed the presence of para nitrobenzoate unit

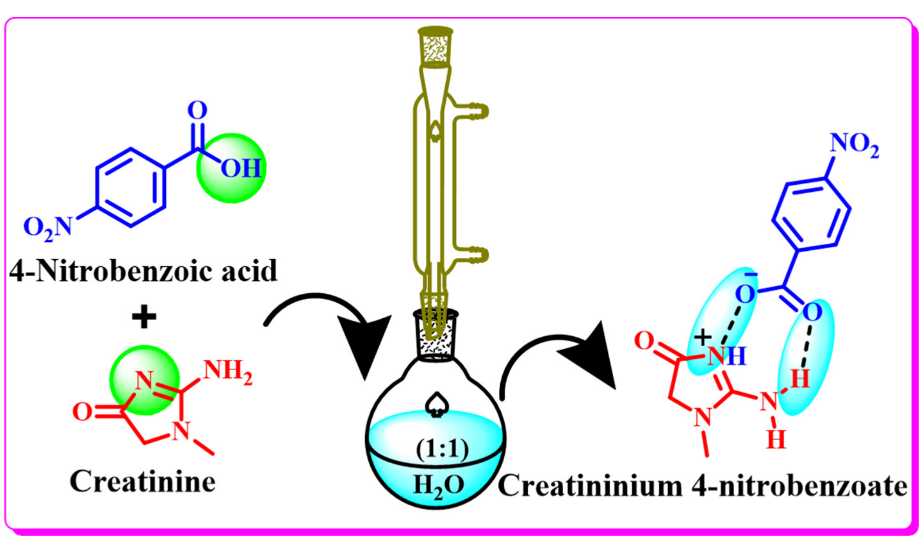

Fig. 1a. Chemical scheme of C4NB compound.

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