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Optical, mechanical and thermal behaviour of Guanidinium Carbonate single crystal

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ABSTRACT

The organic nonlinear optical (NLO) crystals of Guanidinium Carbonate (GC) were grown by the slow evaporation technique. X-ray diffraction studies reveal the tetragonal structure of the grown crystal. The characterization analysis such as powder XRD and Fourier transform infra-red (FTIR) spectral analysis were carried out to find the crystalline nature and the presence of various functional groups in the grown crystal. Further, ultra-violet (UV)–visible spectral analysis, fluorescence study, Differential Thermal Analysis (DTA), Differential Gravimetric Analysis (DGA) and Vickers' hardness were carried out to understand the crystal's optical, thermal and mechanical properties. The nonlinear optical property was confirmed by Kurtz-powder technique and it was found that the second harmonic generation efficiency of the grown crystal is 0.3 times greater than that of the standard KDP.

1. Introduction

Coping with the recent developments, many researchers focusing on new materials which possess high non-linear optical properties owing to their pivotal applications in optoelectronics including optical communications, optical data storage, high speed and information processing, etc. [1–4]. The organic NLO crystals have more advantages than inorganic materials due to their tailor-made flexibility, large band gap, high nonlinear coefficients and appreciable laser damage threshold [5,6]. Guanidinium is a strong base material, easily reacts with most of the organic acids and gives the good crystalline product because of their six potential donor sites for hydrogen bonding interaction [8].

In this present investigation, as an attempt of first kind, we wish to harvest good quality and transparent single crystals from the slow evaporation technique [7]. The structural, optical, thermal, mechanical, fluorescent and NLO properties of Guanidinium Carbonate crystals were investigated and their results were also presented.

2. Experimental procedure

2.1. Crystal growth

The commercially available Guanidinium Carbonate salt (AR Grade) was taken as raw material for growth of crystal and it was dissolved in double distilled water and stirred well for 6 h using temperature controlled magnetic stirrer to obtain saturated solution. Then the saturated solution was filtered using Whatman filter paper and poured in a well cleaned Petri dish for synthesizing process. The synthesized salts were purified by repeated recrystallization and at last good transparent colourless single crystals were harvested after 45 days and are shown in Fig. 1.

2.2. Characterization

The single-crystal XRD and the powder XRD data of the grown GC crystals were recorded using ENRAF NONIUS CAD4 diffractometer with MoKα (λ = 0.71073Å) and Rich-Seifert powder diffractometer with CuKα, respectively. The FTIR spectrum was recorded in the range 400–4000 cm^{-1} by Perkin-Elmer spectrometer (KBr pellet technique). The UV–visible spectrum of GC crystal was recorded between 190 and 1100 nm using Lambda 35 UV-visible spectrometer. The fluorescence spectrum was recorded using SMOOTH10 SP spectrofluorometer in the wavelength range 240–800 nm. TGA and DTA were carried out using SDT Q600 V8.3 Build 101 thermal analyzer in the nitrogen atmosphere at a heating rate of 20 °C/min. The quantitative measurement of the relative second harmonic generation (SHG) efficiency of the grown crystal was made by the Kurtz and Perry powder technique. The detailed results are presented in the following sections.

3. Results and discussion

From the single crystal XRD analysis, it is confirmed that GC crystal belongs to tetragonal system and unit cell parameters

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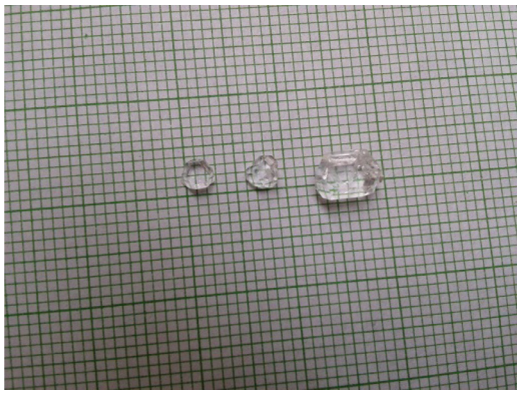

Fig. 1. As grown GC single crystals of GC.

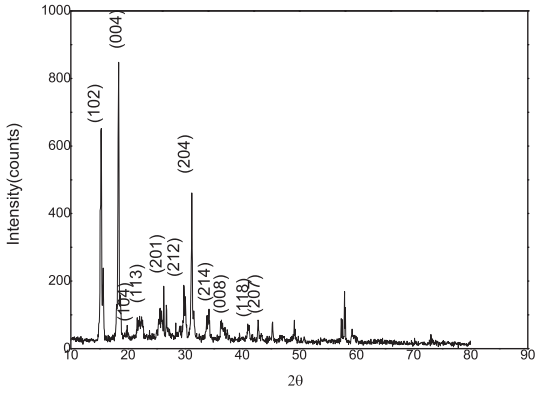

Fig. 2. Powder XRD pattern of GC.

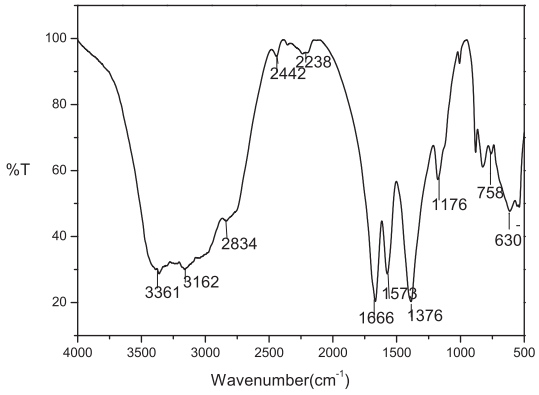

Fig. 3. FTIR spectrum of GC.

are $a = 6.9651$ Å, $b = 6.9731$ Å, $c = 19.5692$ Å and $V = 950.4250$ (Å)^3 with $\alpha = \beta = \gamma = 90^\circ$. These values are in good agreement with the reported values [9]. The powdered sample of the grown crystal was subjected to powder crystal X-ray diffraction to confirm the crystalline nature of the grown crystal and it is evident from the sharp peaks as in Fig. 2.

3.1. Fourier transform infra-red analysis

The FTIR spectrum of GC is shown in Fig. 3. The peaks observed at 3361 and 3162 cm^{-1} are due to the symmetric N—H···O stretching band. The sharp peak at 1666 cm^{-1} is due to the NH_2 bending mode [8]. The attributed peaks at 1573 and 1386 cm^{-1} are due to an asymmetric and symmetric vibration of C=O. The peak at

Table 1
Functional group assignments.

Wave number (cm^{-1})	Assignments
3361	N—H···O stretching
3162	N—H···O stretching
1666	NH_2 bending vibration
1573	C=O asymmetric stretching
1388	C=O symmetric stretching
1176	NH_3 rocking
613	NH_2 rocking

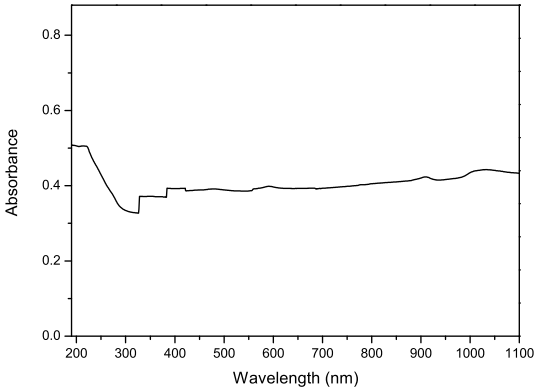

Fig. 4. Absorption spectrum of GC in the range of UV–vis–IR.

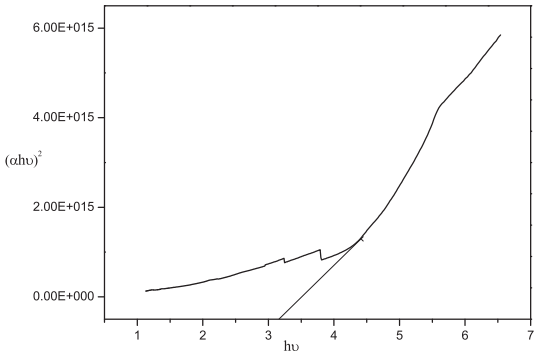

Fig. 5. $ln((\alpha h\nu)^2)$ versus $(h\nu)$.

613 cm^{-1} indicates the rocking mode of NH_2 [10]. The presence of all functional group of GC crystal is shown in Table 1.

3.2. Optical transmission studies

The optical transmittance spectrum of the grown crystal is shown in Fig. 4 and from the UV transmission data, the optical absorption edge, the type of transition of an electron from valence band to the conduction band of this material, optical energy gap, refractive index, reflectance and extinction coefficients were calculated.

The absorption coefficients were calculated using the following relation

$$\alpha = 2.303 \frac{\log(1/T)}{t} \quad (1)$$

where t is thickness and T is the transmittance of the crystal.

By plotting $(\alpha h\nu)^2$ as a function of $(h\nu)$ as shown in Fig. 5 and extrapolating the linear regions of this curve to $(\alpha h\nu)^2 = 0$, we obtained the optical band gap of the grown crystal as 3.16 eV.

The absorption coefficient related to photon energy is

$$\alpha h\nu = \beta(h\nu - E_g)^n \quad (2)$$