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Research Article

INVESTIGATION ON GROWTH, THERMAL, STRUCTURAL, SPECTRAL, OPTICAL AND MECHANICAL PROPERTIES OF ZNS DOPED GLYCINIUM TRICHLOROACETATE CRYSTALS

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ABSTRACT

Optically quality Single crystal of ZnS Doped GTCA were grown from aqueous solution employing slow evaporation technique. From the Powder X-ray diffractograms it is found that ZnS Doped GTCA belongs to Triclinic System. The Lattice Parameters were determined from Single crystal X-ray diffraction analysis. The various Functional groups present in the grown crystals were identified using FT-IR and FT-Raman Spectroscopic analysis. The transmittance and absorbance of electromagnetic radiation is studied through UV-Visible Spectrum. The Thermal behavior of the grown crystals has been investigated by TG/DTA analysis. The emission of green light with the use of Nd:YAG laser (λ=1058)nm confirmed the second harmonic generation properties of the grown crystals. The determined Vicker's hardness number and work hardening co-efficient of the grown crystals ascertains the nature of the crystal.

INTRODUCTION

Nonlinear optical properties are a sensitive probe of the electronic and solid-state structure of organic compounds and as a consequence find various applications in many areas of optoelectronics including optical communications, laser scanning and control functions, and integrated optics technology. Nonlinear optical (NLO) materials are used in optical computing, optical communication, harmonic generators, medical diagnostics, frequency mixing and optical switching (J.Lin *et al*, 1999; P.N.Prasad *et al*, 1991; M.Iwai *et al*, 1997). The search for large second –order electric susceptibilities (that is, proportional to the square of an applied electric field) has concentrated on acentric organic or organometallic chromophores with an organic π-electron system coupling electron donor and acceptor groups. (W.M.Laidlaw *et al* 1993). The key factor for material selection depends on the physical properties of the crystals and the jprospects of their various applications. Specificially, amino acid and strong inorganic acids are good raw materials to produce semi-organic crystals, because amino acid crystals have good optical properties such as optical modulation, frequency shifting, and optical data storage for developing technologies in telecommunications and signal processing (C.C.Frazier *et al* 1987; S.B.Manoco *et al* 1987; P.Gunter *et al* 1997). Amino acids are interesting materials for NLO applications as they contain donor carboxyl acid (COOH) group and the proton acceptor amino (NH_2) group in them. Hydrogen bonds have also been used in the possible generation of noncentrosymmetric structures, which is a prerequisite for an effective SHG crystal (G.R.Desiraju *et al* 2002); D.Xue *et al* 1999); Z.Latajka *et al* 2009). Trichloroacetic acid forms crystalline complexes with amine and amino acids .(J.baran *et al* 2000).

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In the present work, the title compound has been synthesized using slow evapouration technique. The grown crystals were subjected to various characterizations such as single crystal X-ray diffraction studies, Powder X-ray diffraction studies, Fourier Transform Infrared (FTIR) analysis, Optical absorption studies, Microhardness studies, Thermal studies, Nonlinear optical studies were discussed in detail.

Experimental Procedure

The entitled crystal has been grown by slow evaporation solution growth method. The GTCAZS was synthesized from Glycine and Trichloroacetic acid doped with zinc sulphide. The glycine and trichloroacetic acid were taken in equimolar ratio 1:1. The reactants were stirred continuously using magnetic stirrer in double distilled water, after reaching saturation condition the solution was filtered using filter paper and perforations were made for slow evaporation. The seed crystals were obtained after 17 days, recrystallization process was carried out to obtain bulk crystal.

RESULTS AND DISCUSSION

Powder X-Ray Diffraction Study

To ensure the good crystalline nature of the powdered sample the X-ray powder diffraction technique, using PANALYTICAL X-ray diffractrometer with CuKα (λ=1.54060 Å) radiation. Finely crushed powder of GTCAZS Crystal was scanned , the scanning rate was maintained at 1.6 ° /min over a 2θ range of 10° - 50° employing the reflection mode for scanning. The prominent peaks in the XRD pattern have been indexed. The indexed powder XRD diffractogram of GTCAZS cystals is shown in Fig 2.

Fig 1

Single crystal X-ray diffraction study

The single crystal X-ray diffraction studies were carried out for the confirmation of the crystallinity nature of the synthesized sample and the lattice parameters were determined by using ENRAF NONIOUS CAD4-F single crystal diffractometer. The single crystal X-ray diffraction studies confirm the triclinic structure and the crystal lattice parameter values are listed in the Table 1.

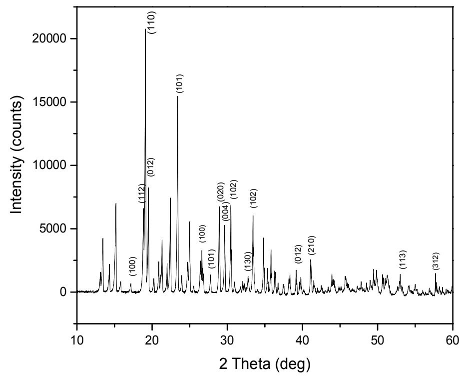

Fig 2 Powder XRD Pattern of GTCAZS crystal.

Table 1 Lattice parameter of GTCZS crystal

Lattice parameter	GTCAZS
a (Å)	5.974
b (Å)	6.836
c (Å)	13.325
α (°)	85.08
β (°)	83.19
ν(°)	82.84
V (A^3)	534.7

UV-Vis spectral studies

The Interaction of light radiation in the entire range of electromagnetic spectrum shows the optical behavior of the material. The optical absorption spectrum for the grown crystals was recorded in the range 200-800 nm using Perkin Elmer Lamba 35 UV/VIS spectrometer. The grown crystals shows good transmittance over the UV and visible regions (269-720nm). The lower cutoff wavelength is around 285nm Fig 3. The Π electron dislocation is responsible for absorption in near UV region. (V.Sheelarani *et al* 2014). This transmittance studies confirms the colourless nature of the crystals. Higher transmittance in the visible region favours the existence of non-linear optical property and suitable for optoelectronic devices fabrication.

The energy band gap has been calculated and the graph is plotted between the energy (hν) Vs $(\alpha h\nu)^{1/2}$ and its shown in the Fig 4. From the plot the energy band gap was found to be 3.88 eV. The absorption coefficient (α) and the extinction coefficient (K) have been determined from the transmittance (T) spectrum based on the following relations,

$$\alpha = \frac{2.3026}{t}\log\left(\frac{1}{T}\right)$$

T- transmittance and 't' is the thickness of the crystal. The absorption coefficient 'α' is related to the extinction coefficient K by is shown by Fig 5,

$$K = \alpha\lambda/4\Pi \, .$$

Ftir Analysis

The FTIR analysis were carried out to confirm the functional groups in GTCAZS. The FTIR spectrum has been recorded in the range 400-4000 cm^{-1}using Perkin-Elmer grating infrared spectrometer is shown in the Fig 6 From the spectrum the observed 3424 cm^{-1} assigned to be symmetric stretching vibration, a weak band obtained at 3071 cm^{-1} is due to NH_3^+ strong stretching vibration, the strong peak at 1735 cm^{-1} confirms the C=O stretching (M.Esthaku Peter *et al* 2012),the absorption at 779 cm^{-1} is due to the presence of carbon-chlorine bond (M.Esthaku Peter *et al* 2012). At 1545 cm^{-1} NH_2 wagging occurs, the sharp strong rocking vibrations are observed at 928 cm^{-1} , the weak C-H bending occurs at 1469 cm^{-1} respectively.

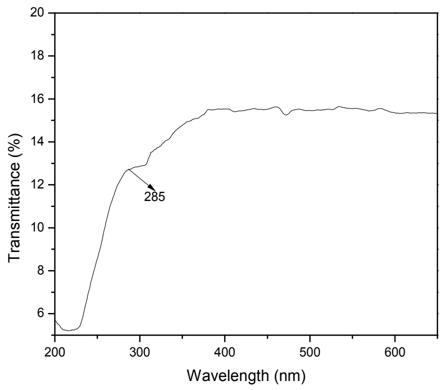

Fig 3 UV-VIS transmission spectra of GTCAZS crystal.

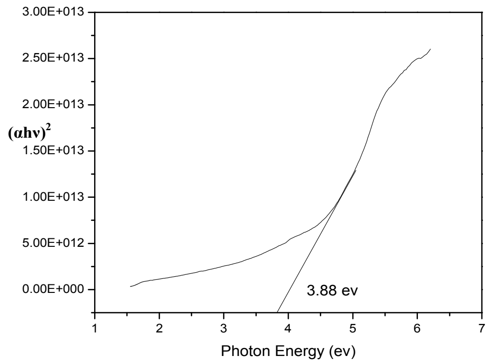

Fig 4 $(\alpha h\nu)^{1/2}$ Vs ($h\nu$) Optical Band Gap

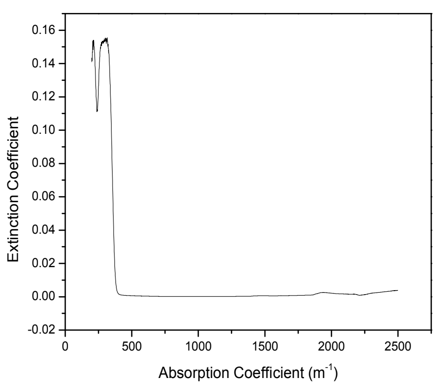

Fig 5 Extinction Coefficient spectrum

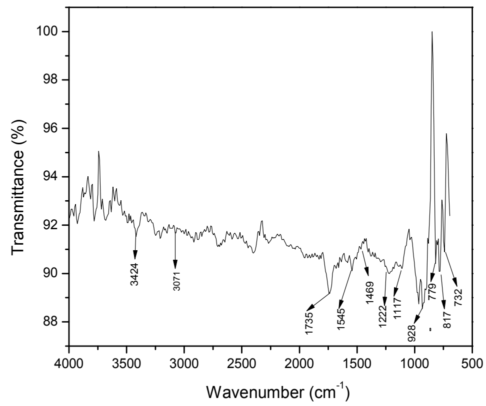

Fig 6 FTIR spectrum of GTCAZS crystal.

Table 2 Frequencies of the fundamental vibrations of GTCAZS crystal

Freuency in Wavenumber (cm^{-1})	Modes of Vibration
3424 (m)	N-HSymmetric stretching
3071 (w)	NH_3^+ Strong Stretching
1735 (s)	C=O Symmetric Stretching
1545 (s)	NH_2 wagging
1469 (w)	C-H Bending
1222 (w)	O-H Deformation vibration
1117 (w)	C-N Stretching
928 (s)	CH_2 Rocking vibrations
817 (s)	N-H Wagging
779 (s)	C-Cl Stretching
732 (s)	CH_2 rocking

Microhardness studies

The Vicker'smicrohardness (Hv) were carried on the grown crystal fitted with diamond indentor. By varying the loads from 25 g to 100 g. The Vicker's hardness number (Hv) values at different loads were calculated using the expression
$Hv= 1.854\ (P/d^2)\ Kg/mm^2$

P-applied load on the indentor in g and d is mean diagonal length of the square impression formed on the crystal surface in µm. As load increases there is an increase in the hardness number. The plot of log P versus log d for the grown crystal is shown in Fig 7. The slope gives the work hardnening index n, and is found to be 1.23, shown in the Fig 8.

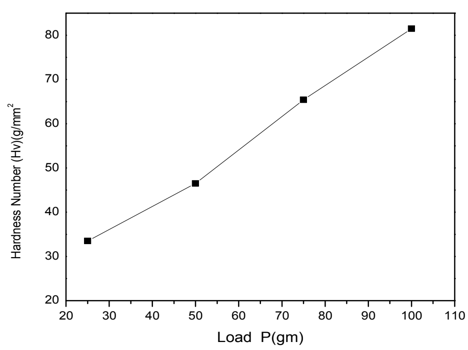

Fig 7 LoadVs Hardness number.

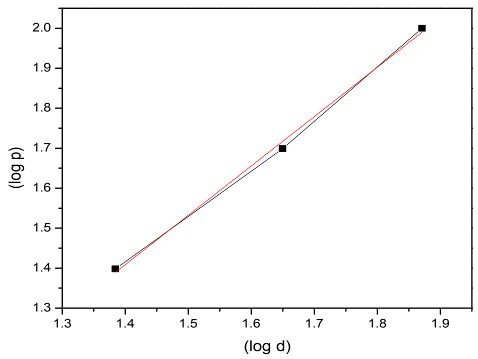

Fig 8 log P Vs log d

Thermal Analysis

Thermal analysis were carried out on the grown crystal to study the thermal stability and melting point. The TGA and DTA were carried for the sample weight of 8.274 mg between the range of room temperature (30 °C) and 300 °C at the heating rate of 10 °C per min. The analysis was performed in nitrogen atmosphere using alumina thermal analyzer. In DTA curve two weight loss begins around 79.9 °C the loss of weight corresponding to decomposition of the given sample was observed around 134.3 °C. The second peak corresponds to endothermic transition in the DTA curve explicits the material was fully decomposed by at 134.3 °C, shown in the Fig 9.

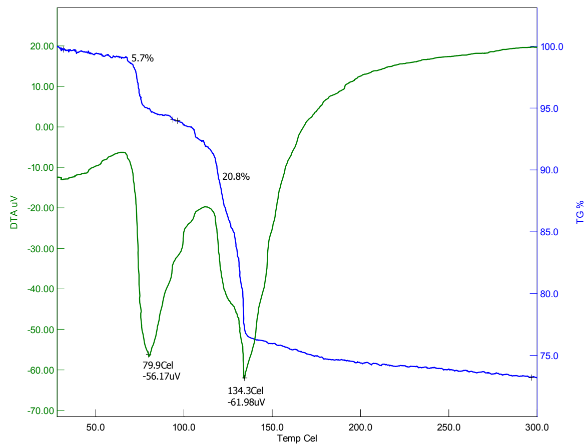

Fig 9 TG/DTA spectrum of GTCAZS crystal.

Nlo Studies

The Second Harmonic Generation (SHG) conversion efficiency of the grown crystal was carried out using the Nd:YAG laser beam of wavelength 1064 nm, producing pulses with a width of 8ns and the repetition rate is 10 Hz using Kurtz powder technique (kurtz *et al*, 1968). The second harmonic generation was confirmed by the emission of green radiation of wavelength of 532 nm and NLO efficiency is found to be 0.74 times that of KDP.

CONCLUSION

The GTCAZS crystal has been grown using slow evaporation technique from the saturated solution. From the optical transmittance studies the grown crystal has good transmission in the entire visible region and the lower cutoff wavelength was found to be 285 nm, which is important parameter for the fabrication optoelectronic devices. The band gap was found to be 3.88 eV. The FTIR analysis confirms the presence of functional groups in the grown crystal. The thermal stability of the grown crystal were obtained by TG/DTA curves and the crystal was found to be thermal stable upto 134° C. The mechanical strength of the grown crystal was determined by vicker's hardness test and the hardening coefficient was determined as 1.23. Hence from these various analysis it was found to be well suitable for the fabrication of optoelectronic devices.

Reference

1. J.Lin, M.H. Lee, Z, Liu, C, Chen, C.J. Pickard, Phys. Rev. B 62 (1999) 13380.
2. N. Prasad, D.J. Williams, Introduction to Nonlinear Optical Effects in Organic Molecules and Polymers, Jhon-Wiley & Sons Inc., New York,1991.
3. M.Iwai, T.Kobayashi, H.Furuya, Y.Mori, T.sasaki, *Jpn.J.Appl.Phys*.36 (1997)76.
4. W.M.Laidlaw, R.G.Denning, T.Verbiest, E.Chauchard,. Persoons, *Nature* 363(1993) 58.
5. C.C.Frazier, M.P.Cockerhamn, E.A.Chauchard, C.H.Lee, *J.Opt.Soc.Am.B4* (1987)1899.
6. S.B.Monaco, l.e.Davis, S.P.Velsko, F.T.Wong, D.Eimerl, *J.Cryst.Growth* 85 (1987)252.
7. P.Gunter, Ch.Bosshard, K.Sutter, H.Arend, G.Chapuis, R.J.Twieg, D.Dobrowolski, *Appl.Phys.Lett*.50 (1997) 486.
8. G.R.Desiraju, *Acc.Chem.Res*.35 (2002) 565.
9. D.xue, S.Zhang, *Chem.Phys.Lett*. 301 (1999) 452.
10. Z.Latajka, G.Gajewski, A.J.Barnes, D.Xue, H.Ratajczak, *J.Mol.Struct*.928 (2009)
11. J.Baran, A.J.Barnes, B.Engelen, M.Panthofer, A.pietraszko, H.Ratajczak, M.Sledz, *J.Mol.Struct*. 550-551 (2000) 41.
12. V.Sheelarani, J.Shanthi, IJRSR, Vol 5, 6, pp. 1116-1118, June, 2014.
13. M.Esthaku Peter, P.Ramasamy, *Materials Chemistry and Physics* 137 (2012) 258-263.
14. H.S. Randhawa, Modern Molecular Spectroscopy, macmillan India Ltd, 2003.
15. John Coats, Interpretation of Infrared Spectra, a Practical Approach, John Willey & Sons Ltd, Chicheser, 2000.

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