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Synthesis, Crystal, Growth and Characterization of L-Tyrosine Guanidine Carbonate Single Crystal Single Crystal

L .Anandaraj, S. Diviya Priya , T. Naveenkumar*

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Abstract

A new Non-linear optical material L-tyrosine Guanidine Carbonate single crystal is synthesized by slow evaporation solution growth technique at room temperature using water as solvent. Good transparent LTGC crystal is sized. Single crystal X-ray diffraction reveals the crystal belongs to the Tetragonal P structure and a space group of P41212. The sharp intense peak in Powder XRD analysis confirms the good crystalline nature and purity of the crystal. The presence of various functional groups and their modes of vibration were identified by FTIR spectral analysis. The UV-Vis spectroscopic study shows that the lower cut-off wavelength is 234.6 nm with wide transparency range and very low absorbance. The optical band gap spectrum shows the Energy gap of the crystal is about 5.6 eV. The LTGC was subjected to fluorescence analysis and it was ascertained that the maximum emission was in green region at 532.4 nm. The mechanical behavior was studied by Vickers microhardness test.

Keywords: Single crystal XRD, Microhardness, Fluorescence.

1. Introduction

The researchers are encouraged in the recent days to grow a nonlinear optical (NLO) material due to their high optical transparency, high laser damage threshold, extremely high optical response, wide phase angle and high mechanical strength [1]. Wide range of applications in the field of optical switching optoelectronics, optical data storage, optical communication and telecommunication etc., are in the current research of NLO material [2]. For NLO applications the amino acids are interesting organic nonlinear optical material, a compound with improved NLO activity and mechanical, thermal stability is formed when the amino acids are coordinated with strong acids or metallic bonds [3]. Some organic NLO materials having less environmental stability, poor optical and mechanical property, low laser damage threshold and poor phase matching property due to their weak Vander Waal bonds. The growths of semi-organic crystal were used to overcome this difficulty second order optical non-linearity, high transparency range, high nonlinear co efficient, high mechanical stability and high laser damage threshold etc. [4]. By slow evaporation method the semi-organic crystal was grown and which is crystallized by monoclinic system

***Corresponding author:** E-mail: anandaraj1828@gmail.com
Affiliation: Department of Physics, Sacred Heart College (Autonomous), Tirupattur-635 601, Tamil Nadu, India.

with non-Centro symmetric space group P41212. KDP, Zno4 doped Zno4 are inorganic materials potassium lithium niobite, are niobite crystals borate crystals like lithium triborate have been already reported to NLO active materials. Materials like glycine selenite proves to be highly NLO active. Lithium sulphate family are excellent NLO materials also many new crystals in the material. Compounds is already reported and the title is detailed structure and analyzed [5]. Remarkable changes in the properties of inorganic crystals recently it confirmed that the effect of dopants. The properties of the material such as transparency, reflectance, refractive index, optical electrical conductivity, electrical susceptibility, dielectric constant, Mayer's number, stiffness constant, yield strength, fracture toughness and brittle index is varied by adding dopants to the undoped inorganic crystals. In advanced laser technology and telecommunication applications the ferromagnetic and nonlinear optical material plays a huge role. In the field of electronic industries, the NLO material have a vast range of demand, so to enhance the properties of a material it is require to synthesis a new NLO. Considering all the above facts, L-tyrosine and guanidine carbonate single crystals have been synthesized and grown at low cost. L-tyrosine, a natural amino acid, is a major nutrient having a phenolic hydroxyl group [6]. L-tyrosine is a centrosymmetric molecule, when coordinated with metal ions it becomes non-centrosymmetric materials and these metal-organic coordination compounds have attracted attention for their considerable high NLO coefficients, favor physico-chemical properties [7]. Guanidine is a strong base that readily protonated by most organic acids with the resulting guanidine species being useful for molecular assembly purposes, forming hydrogen bonding associations through its six donor protons . The grown crystal was subjected to powder X-ray diffraction due to the single crystal X-ray diffraction the crystalline system and space groups are determined and the functional groups are analyzed with help of FTIR. Using a UV-Visible analysis, the optical transmission and optical absorption was studied and the fluorescence study exhibits that material having a green color emission.

2. Experimental procedure

The L-tyrosine was prepared in an equimolar ratio of 1:1, diluted in distilled water using a magnetic stirrer and filtered through Whatman filter paper. Guanidine carbonate, on the other hand, was produced at an equimolar ratio of 1:1 and dissolved in distilled water using a magnetic stirrer before being filtered through Whatman filter paper [8]. The filtered L-tyrosine and Guanidine carbonate solutions were then combined in a single beaker and agitated for 1 hour before being filtered again with Whatman filter paper. For the slow evaporation procedure, the solution was held at a steady temperature.

3. Characterization studies

3.1. Single crystal XRD

Single crystal XRD studies are carried out to obtain reliable details on lattice characteristics that are comparable to powder XRD research. For the xrd analysis and cell parameter calculations, a fitting crystal size was chosen

[9]. The Tetragonal P system is associated with L-tyrosine and Guanidine carbonate crystals, according to a single XRD result. Bruker D8 VENTURE SC-XRD equipped with MoKα radiation was used to collect the unit cell dimensions and X-ray intensity data of LTGC (8). The crystal belongs to the Tetragonal P structure, with unit cell dimensions of a=6.982 Å; b=6.982 Å; c=19.635 Å; α=90°; β= 104.24°; γ=90° and a space group of P41212 Volume 957.173 $Å^3$.

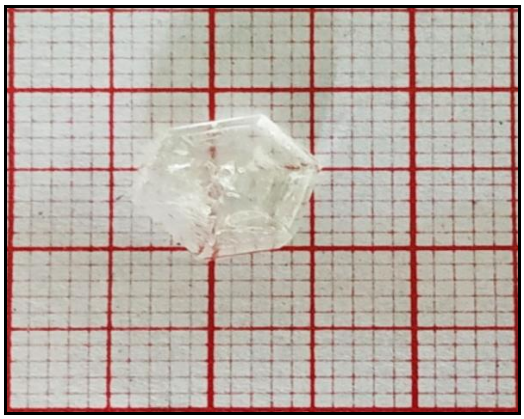

Fig.1.Photograph of L-tyrosine Guanidine carbonate single crystal

3.2 Powder XRD analysis

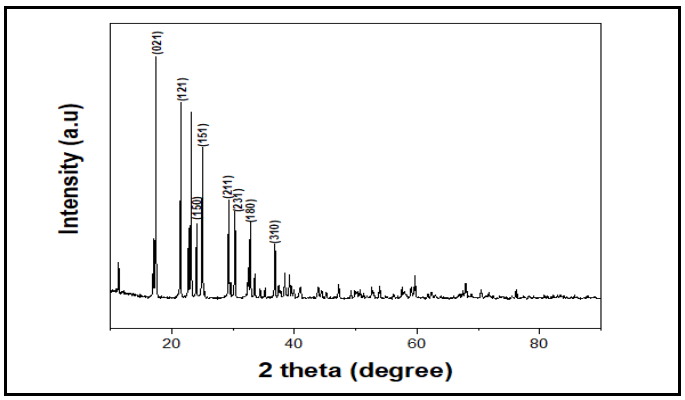

Fig.2. Powder X-Ray diffraction pattern for LTGC

Powder XRD was performed on L-tyrosine and Guanidine carbonate crystals using a Rich Seifert diffractometer with CuK radiations of wavelength 1.5418 [10]. The powder XRD pattern of LTGC is shown in the figure 2. The peaks detected in the XRD spectrum were analyzed and indexed, and the produced crystals belong to the orthorhombic system, with the computed lattice parameters agreeing well with the data acquired from a single XRD.

3.3. FTIR Analysis

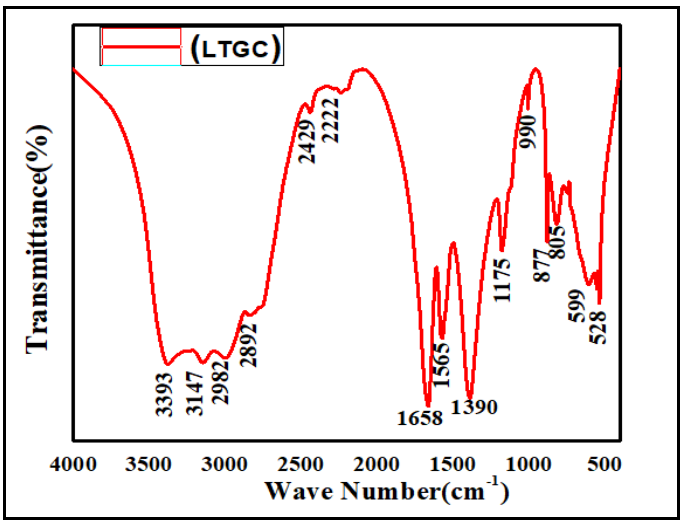

Fig.3. FTIR spectrum of LTGC

Spectral analysis is used in Fourier Transform Infrared spectrometers to analyses molecule structure and chemical bonding. 3000 cm^{-1} – 2500 cm^{-1} stretching vibration of OH band in H_2O absorbed by a sample can be attributed to the sample that occurs at the peak. The peak is attributed to the stretching vibration CH_2 band at 2441 cm^{-1} and 2239 cm^{-1}. The carbonyl stretching vibration of (C(N)=0) bands produces the peak attributed to 1665 cm^{-1}.

For all peaks present in the FTIR spectrum, the respective assignments of their functional groups are tabulated in the below table 1. For all peak values, their bending and stretching vibrations confirm its presence.

Table 1 : FTIR Assignments

S.No.	Wave Number (cm^{-1})	Functional group
1	528	C-C-C (Bending)
2	805	NH_2 (Stretching)
3	877	CH_2 (Stretching)
4	990	CH (Stretching)
5	1390	OH (Bending)
6	1658	(C(N)=O) (Carbonyl Stretching)
7	3147	OH (Stretching)

3.4 UV-Visible spectral analysis

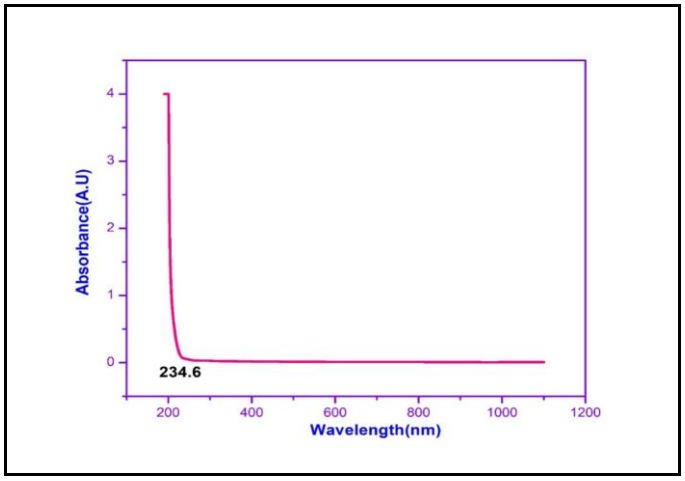

Fig.4. UV-Visible Absorbance spectrum of LTGC

The absorbance of L-tyrosine and Guanidine carbonate crystal is shown in the diagram above. In the region of 200-1200 nm, the L-tyrosine and Guanidine carbonate crystal absorbs light [11-13]. The lower cutoff wavelength for the absorption spectrum is 234.6 nm. The spectrum demonstrates that it will absorb a specific wavelength of light from the source while transmitting all other visible wavelengths. The crystal's low absorption indicates that it can transmit a laser beam in the 200-1200 nm range. It demonstrates the crystal's transparency.

3.5 UV -Visible band gap spectrum LTGC crystal

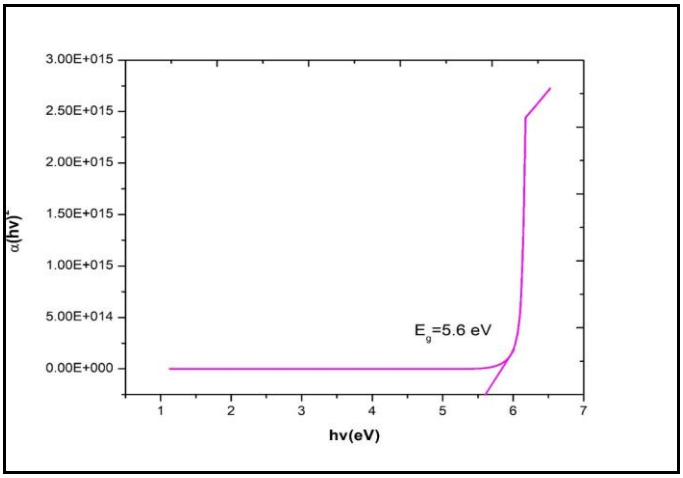

Fig.5. UV-Visible spectrum of band gap for LTGC

The wavelength of the optical cut-off is found to be 234.6 nm. We may use the formula to get the absorption coefficient using that cut-off wavelength value.

$$\alpha = 2.3023 \log/ t$$

where, α – absorption co-efficient, T – transmittance, t – thickness of the crystal. The band gap of a LTGC crystal is determined by using a following relation,

$$Eg = (\alpha h\nu)^2/h\nu$$

The LTGC crystal has a large optical band gap of 5.6eV, making it appropriate for optoelectronics applications.

3.6 Fluorescence Study

L-tyrosine and Guanidine carbonate crystals were identified from the fluorescence spectrum. With the help of a VARIAN CARY ECLIPSE fluorescence spectrometer, the sample is placed at ambient temperature. The fluorescence

emission spectra were measured in the 500-700 nm range [14].

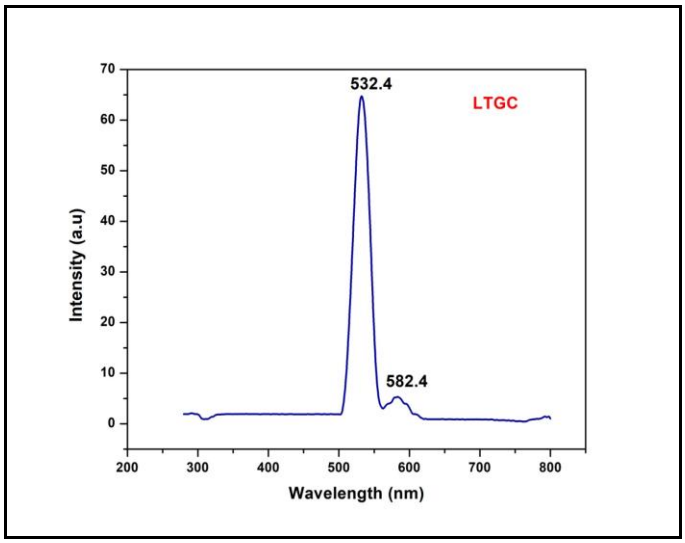

Fig.6. Fluorescence study of LTGC

The big peak and the tiny peak are both GREEN in color. The tiny peak's range is around 582.4 nm, while the high peak's range is around 532.4 nm.

3.7 Micro Hardness Analysis

A micro hardness tester is used to investigate the mechanical properties of the LTGC single crystal. The hardness of a material is a measure of its resistance to deformation[15,16].

The micro hardness characterization is just as important as the device fabrications, and this investigation of the produced LTGC crystals was done at room temperature using the Vickers hardness test. The generated crystal's Vickers hardness number was estimated using the formula $Hv = (1.854P)/d^2$ Kg/mm^2. Where Hv is the Vickers hardness number in kilograms per square meters, and Kg/mm^2 is the Vickers hardness number in kilograms per square metre.

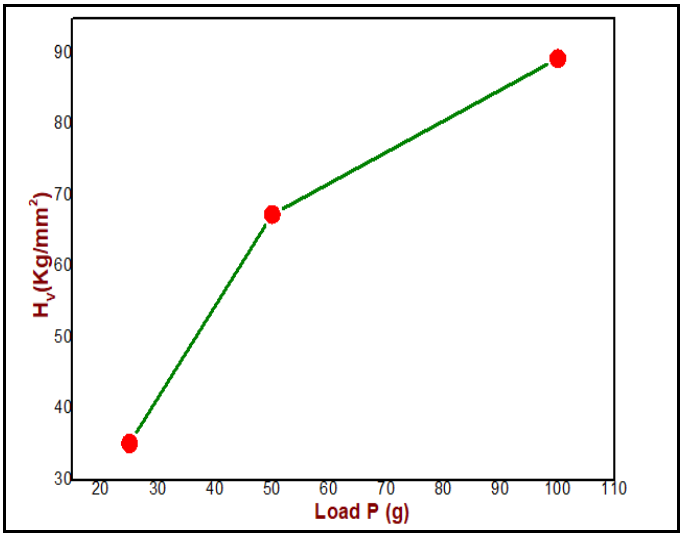

Fig.7. Load P and Vs Hardness number of LTGC

P denotes the applied load in kilograms.

D is the indentation mark's average diagonal length in millimeters. The hardness number (Hv) and the applied load P were shown on a graph. The graph shows that the value of toughness increases as the number of people increases.

4. Conclusion

A new nonlinear semi – organic material of L–tyrosine with Guanidine carbonate was synthesized by slow evaporation method. The functional group and molecular structure of the material was concluded by FTIR analysis. The single crystal XRD confirmed that the grown LTGC crystal was said to be TETRAGONAL P system and it exhibit a P41212 space group and lattice parameters a=6.982Å, b=6.982Å and c=19.635Å. The UV cutoff wavelength was found to be 234.2 nm and it shows that material has a good candidate of NLO. The emission spectrum of LTGC is around 532.4 nm which exhibit a Green color emission.

Conflicts of Interest

The authors declare that they have no known conflicts of interests.

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