Volume-04
Issue-03
March-2019

ISSN: 2455-3085 (Online)
RESEARCH REVIEW International Journal of Multidisciplinary
www.rrjournals.com[UGC Listed Journal]

# Effect of L-Threonine Doping on Optical, Structural and Thermal properties of KBr Single Crystals

[1]B.Ravindran, [2]T.Manimaran, [3]S. Bhuvaneswari and [4]N.Chandrasekaran, [5]S.Kamali

*[1]AssistantProfessor,PG&ResearchDepartment of Physics Thiru. Vi.Ka. Government Arts College, Tiruvarur (India)*
*[2,3,4]Research Scholar, PG & Research Department of Physics Thiru. Vi.Ka. Government Arts College, Tiruvarur (India)*
*[5] Assistant Professor, University College of Engineering, Thirukkuvalai Campus (India)*

**ARTICLE DETAILS**

**Article History**
*Published Online:* 13 March2019

**Keywords**
UV, FTIR,TG-DSC,XRD,SHG

***Corresponding Author**
*Email: ravitvk74[at]gmail.com*

**ABSTRACT**

A new NLO crystal L-Threonine doped Potassium Bromide (LTPB) crystal is reported by synthesis and growth along with the comparison of pure L-Threonine. Grown crystals of LTPB crystals are characterized with UV-Vis-NIR, FTIR, Powder XRD, TG-DSC, and SHG. Clear crystals of very good transparency were harvested by slow evaporation technique at room temperature. Inclusion is confirmed with the change in the structure of materials using Xrd pattern. FTIR spectrum exposes the available functional groups in the grown crystal to confirm the new arrival. TG-DSC spectra show the thermal properties of LTPB found that the thermal stability extends up to 750°C. The basic optical behavior of the grown crystal was examined using absorption and transmittance spectra obtained from UV-Vis-NIR spectra. The efficiency of SHG of the LTPB crystal was recorded using Kurtz powder method.

## 1. Introduction

Impact on the applications in communication, laser technology, optoelectronics and industry attracts the interest of researchers for the past few decades. Current research is going on to fabricate THG crystals to satisfy future needs. Number of researchers was doing research around the world to improve the performance of the Non-linear optical materials. Normally the organic crystals may damage during the process and found to be very poor in mechanical and thermal behavior. It is hard to grown bulk sized crystal for the fabrication of devices. But on the other hand inorganic crystals possess excellent mechanical and thermal properties with poor optical quality because of π-electron delocalization lacking (1). Researchers' interests have been focused on fabricating the semi-organic crystals anticipating the combined favorable properties of both organic and inorganic crystals such as a high laser threshold damage, transparency, chemical strength and stability for advanced device fabrication. Crystal growth and characterization is a vast field and most of the researchers focusing the quality optical crystals due to its broad applications such as optoelectronics and photonics field (2-4) due to the presence of zwitterions and dipolar nature of amino acids.

## 2. Experimental Procedure

### *2.1.Synthesis*

L-Threonine doped KBr crystals have been grown by solution growth slow evaporation method in the aqueous solution at constant room temperature. Continuous stirring of the saturated KBr solution along with the dopant for about 2 hours was done to get the doped homogeneous mixture. Using clean beaker the prepared solution was collected by proper filtering and kept in an undisturbed position by covering the beaker with perforated plastic covers. Within a short span of time (15 days) a good quality single crystal of a predictable size (25 X 23 X 4 mm) was harvested as shown in the figure.

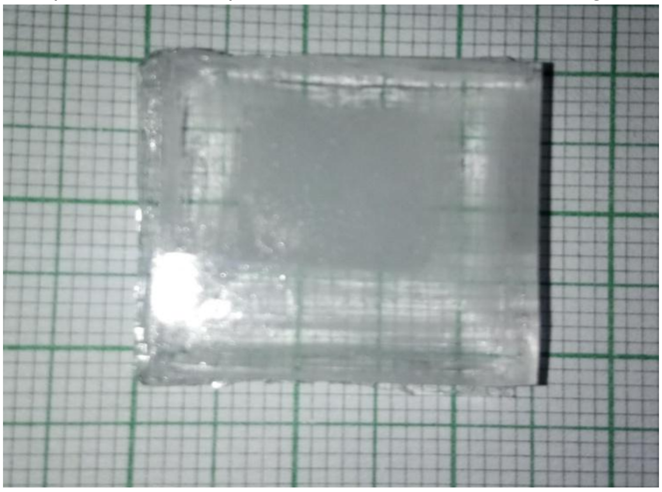


*Fig.1. Photograph of LTPB*

## 3. Results and Discussion

### *3.1.FT-IR Studies*

The Fourier Transfer Infra Red spectrum of LTPB crystals was recorded by Perkin Elmer spectrometer using KBr pellet technique between the frequency ranges from 400-4000cm-1 as shown in the fig.2. Functional groups identification using infrared spectroscopy provides complete information on compared with any other electronic spectra. IR spectrum records the vibrational-rotational spectra. Identification of functional groups in the grown crystal was predicted by the presence or absence of absorptions bands. The L-threonine structure comprises Carboxylic group (COO) and two CH groups, C=O, amine(NH3), two CH groups and CH3. The tentative assignments given in the table1 shows that the KBr molecules would be coordinated with L-threonine and it was confirmed with the major variation of frequencies observed (5).

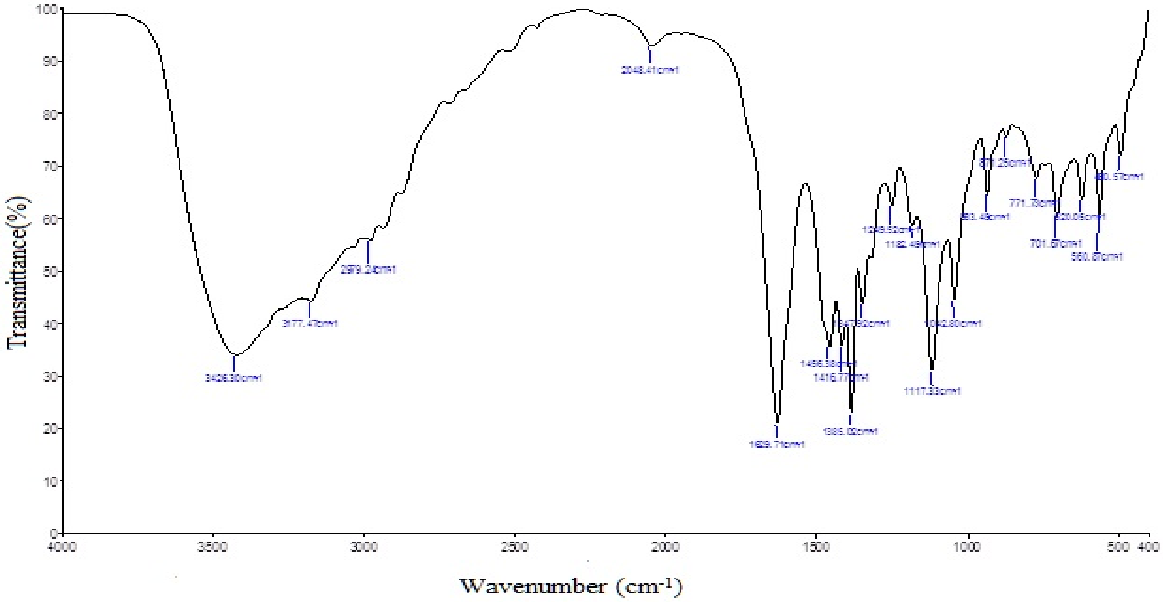



*Fig.2.FT-IR Spectrum LTPB*

**Table. 1. FUNCTIONAL GROUP ASSIGNMENTS OF LTPB**

| LTPB | L-Threonine | Assignments |
|---|---|---|
| 490 | 480 | $NH_3$torsional mode |
| 560 | 558 | $CO_2$- rocking |
| 620 | - | out of plane OCO rocking |
| 701 | - | - |
| 771 | 767 | $CO_2$-bending |
| 871 | 850 | CCN stretching |
| 933 | 928 | C-C stretching |
| 1042 | 1037 | Stretching of CN |
| 1117 | 1111 | $NH_3$ rocking |
| 1182 | 1184 | $NH_3$ rocking |
| 1249 | - | - |
| 1347 | 1346 | $CH_3$ symmetric bending |
| 1385 | - | - |
| 1416 | 1417 | $CH_3$ asymmetric stretching |
| 1456 | - | - |
| 1629 | - | - |
| 2048 | - | - |
| 2979 | - | CH asymmetric Stretching |
| 3426 | - | OH Stretching Vibrations of $H_2O$ |

### *3.2. UV-Vis-NIR Analysis*

Fig.3 shows the UV-Vis-NIR spectrum of LTPB crystals. Using the dual beam spectrometer of Varian Cary 5E model the spectrum was observed and recorded in the range of wavelength 100 to `1000nm. Normally three types of transition are possible (i) π,σ and n electron transitions (ii) charge-transfer electron transitions and finally (iii) d, f electron transitions. Here the lower cut-off wavelength of the grown crystal observed at 249 nm is because of the π –π* transition. The lower cutoff range confirms the suitability of the grown crystals for NLO applications (6). Usually, the organic compounds absorption spectra recorded due to the transition made by π or n electrons to the excited level π*.

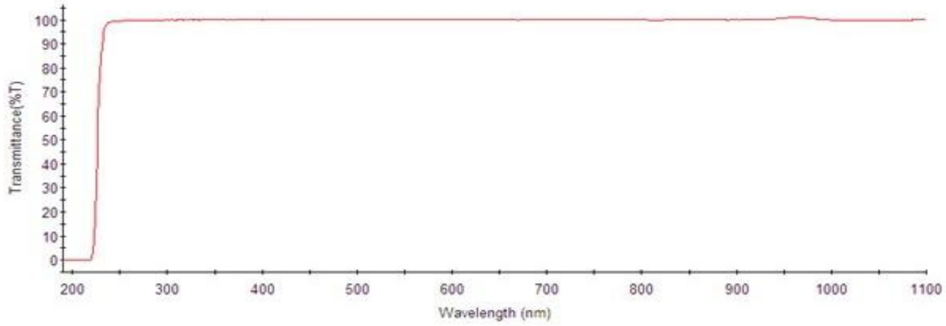
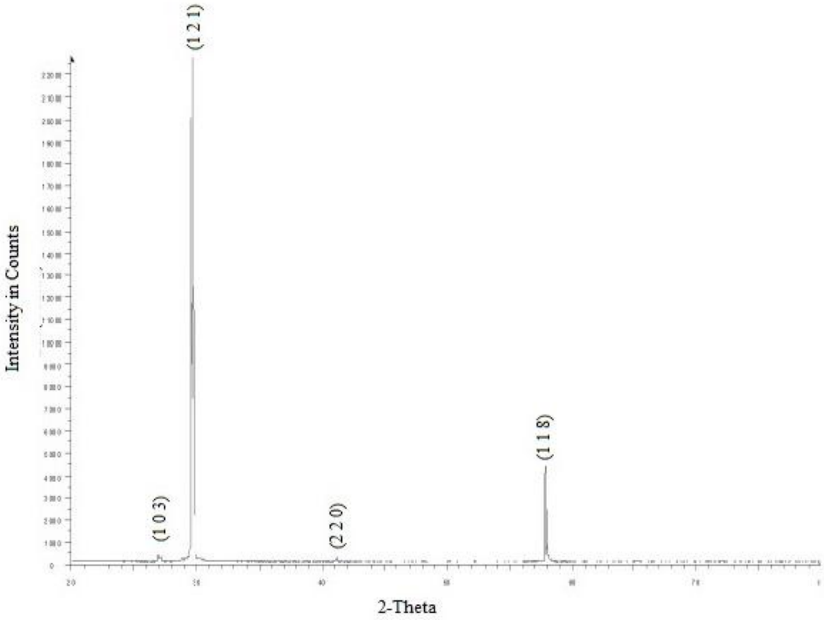



*Fig.3.The UV-visible spectrum of LTPB*

### 3.3. X-ray Diffraction Analysis

Powder XRD patterns of LTPB crystals was recorded using an X-ray diffractometer (JDX8030 Model) with CuKα (λ=1.5408 A) radiation are shown in figure.4. Observed sharp peaks in the XRD pattern shown the inclusion of L-Threonine in the KBr crystals. Powder V1.0 software was used to estimate the corresponding miller indices with the observed 2θ values. The lattice parameters of the grown crystal were also calculated using unit cell software which found to be in good agreement with the reported value (7-8).




*The fig.4.x-ray diffraction pattern of LTPB*

**Table 2.POWDER XRD DATA OF LTPB CRYSTAL**

| 2θ | hkl |
|---|---|
| 26.881 | 103 |
| 29.506 | 121 |
| 41.181 | 220 |
| 57.892 | 118 |

### 3.4. TGA-DSC Analysis

Traces of LTPB crystal is shown in the fig.5. LTPB single crystal was subjected to differential scanning calorimetry (DSC) and thermo-gravimetric analysis (TGA) at a heating rate of 10K/min in a nitrogen atmosphere using NETZSCH STA 409°C/CD instrument. Up to 750°C, no change occurs in the TGA curve predicts that the thermal stability of the grown LTPB crystal is very high and concludes the presence of $H_2O$ molecules. Here the decomposition starts from 750°C. The endothermic peak found at 745°C in the DSC spectrum curve confirms the decomposition starting temperature range and where the heat absorption takes place which shows that the decomposition and melting take place simultaneously. At 840°C, it starts to observe heat and complete decomposition occurred.

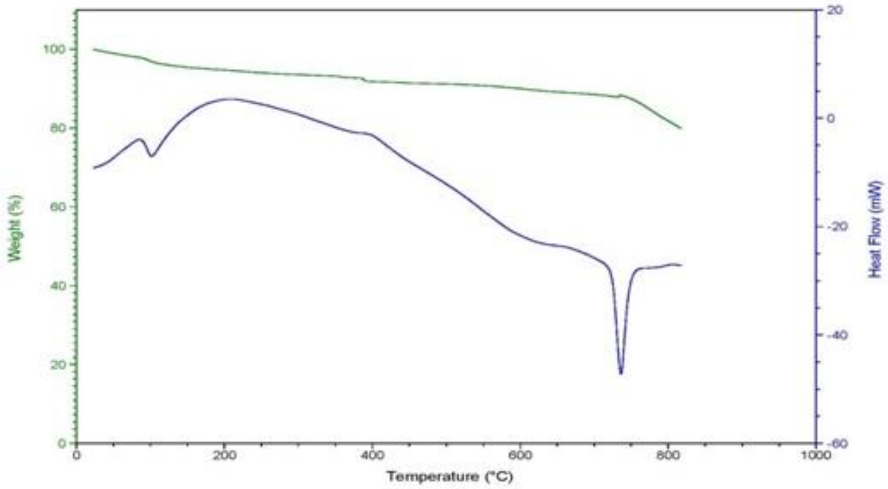



*Fig.5.TGA-DSC analysis of LTPB*

### *3.5. NLO Studies*

SHG efficiency of the grown LTPB crystal was determined using Kurtz and Perry Powder method which is an important method for the evaluation of NLO efficiency. The grown sample was powdered using a mortar and dried using a drier. The dried sample was tightly packed in a fusion tube with a uniform capillary bore. Q-Switched Nd-YAG laser (1064) beam with a power input 2.9mj and 10 ns of pulse width with a repetition rate 10 Hz was made to incident on the prepared sample. The exposed powered sample was illuminated and the emerged beam was made to display in the cathode ray oscilloscope through photomultiplier tube (PMT). The optical signal was converted into electrical pulses by PMT and the same is recorded in CRO (9). Actually, the KBr crystal shows that the NLO efficiency was 1.3 times greater than KDP(10) but on the inclusion of L-Threonine it was found to be recorded 1.9 times of KDP. So it was confirmed that the addition of L-Threonine improves the SHG efficiency of KBr. Hence the grown LTPB crystals may be used for NLO applications device fabrication.

## 4. Conclusion

Single crystals of LTPB with good quality were grown by slow evaporation solution growth technique. The FTIR analysis ascertained the presence of functional groups and confirms the inclusion of L-Threonine. Doping atom incorporation into the host atom was confirmed by the FTIR functional group analysis. Good transparency in the ultraviolet and visible range of the grown crystal was shown in UV-Vis-NIR spectral analysis. The Thermal stability of LTPB crystal was observed up to 750°C a very high range and the crystal may be utilized up to that temperature as operating temperature. SHG efficiency was found to be 1.9 times greater than that of KDP by emitting green radiation from the NLO study. Hence it was concluded that the grown LTPB crystal may play a vital role in the optical device fabrications.

## References


1. M.A.Gaffar,A.Bu El-Fadi,S.Bin Anooz, “Influence of strontium doing on the indirect band gap and optical constants of ammonium zinc chloride crystals,”Physica B,vol.327,pp.43,2003.
2. N.Indumathi,K.Deepa and S.Senthil Growth and Characterization of L-Threonine Lithium Chloride: A New Semiorganic Non-Linear Optical single Crystal 2017IJEDRVol.5,Issue 1pp560-564.
3. D. Kalaiselvi,R.Jayavel,”Synthesis,growth and characterization of L-Proline dimercuric chloride single crystals for frequency conversion applications,” Appl Phys A, vol.107,pp.93-100,2012.
4. R. Subhashini,D.Sathya, V. Sivashankar, P.S.Latha Mageshwari, S. Arjunan.”Growth and Characterization of Bis(L-Threonine)copper(ii) monohydrate single crystals;A Semiorganic second order optical material,”Opt.Mater,vol.62,pp.357-365,2016.
5. Krishnan .R, S, Sankaranarayanan. K and Krishnan K.”Raman and infrared spectra of amino acids.” Journal of the Indian Institute of Science, vol.55,pp:66-116,1973.
6. Senthil Pandian M,Ramasamy P, J Crystal growth, 2010,pp 413-419.
7. Paul Raj and C. Ramachandra Raja Synthesis, Growth, Strutural,Spectroscopic,Thermal and Optical Properties of NLO Single Crystals L-Threonine Zinc Acetate JPO,Vol.2 Issue,3Joly2013pp56-64
8. B.E. Warren, X-ray Diffraction, Addition Welsey,California,1969.
9. Kurtz S.K,Perry T.T,J.Appl Phy.1968,3798,39.
10. J. Uma Maheswari, C.Krishnan,S. Kalyanaraman,Selvaraj,Characterization of KBr crystals grown in the aqueous solution of Picric acid ,Phsica B: Condensed Matter Vol.502,1 Dec 2016,pp32-38.