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Growth and Structural studies of Zn doped L-Threonine single crystal

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----------**ABSTRACT**----------
Non linear optical phenomenon in material plays a major role in the emerging photonics and opto electro technologies. In the search of new and efficient NLO material in organic element (Zn) doped L-Threonine organic crystal were grown in the present study. The grown crystals were characterized by measuring the density by floatation technique. The structure of the crystals were studied by FTIR spectrum. The lattice parameters of pure and doped crystals were calculated from SXRD and PXRD respectively. The lattice parameters shows the crystal belong to orthorhombic system

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I. Introduction

Recently much attention has been paid non-linear optical (NLO) materials mainly because of their interacting potential applications. The compound of this type can be used in LASER technology, optic communication and optical switching. Also, the NLO plays an important role in the merging photonic and opto electronic technologies. The NLO properties of large organic molecules and polymers have been the subject of extensive theoretical and experimental investigations during the past two decades [1]. Organic materials possess several advantages compared with the traditional inorganic NLO materials like ADP, KDP and KTP such as large second harmonic conversion efficiency birefringence and dispersion of refractive index which are finding increase in use in the development of new photonic devices [2]. However, their often inadequate transparency, poor optical quality and lack of robustness, low laser damage threshold and inability to grow to large size have impeded the use of single crystal organic materials in practical device applications. Hence recent research is concentrated on semi-organic materials due to their large non- linearity, high resistance to laser induced damage, low angular sensitivity and good mechanical hardness. L-Threonine is a pure organic material. Mixing of inorganic material may change the quality of the organic crystals. So, In the present study the Zinc Sulphate has been doped instead of mixing in the L-Threonine single crystal to overcome the disadvantage of organic NLO materials. L-Threonine is an important amino acid, which shows higher SHG(Second Harmonic Generation) efficiency than that of many other non linear amino acids. Also it is an important polar amino acid and its dipole moment is nearly similar to water [3]. Several work has been done in L- Threonine single crystal [4-10]. In the present study Zinc Sulphate doped L- Threonine crystal was grown and characterized. The results were discussed here.

II. Experimental Details

Commercially available AR grade L-Threonine, $ZnSO_4$ and doubly distilled water were used to prepare the solution. Saturated solution of L-Threonine was prepared at 35℃ according to the solubility data available in the literature [11]. Pure and ZnS doped L-Threonine single crystals were grown from aqueous solution by slow evaporation technique for the various dopant concentration ratio viz.1:0.002, 1:0.004, 1:0.006, 1:0.008 and 1:0.01. In the present study, totally six crystals were grown. The density of all the grown crystals were determined by flotation technique. Carbon tetra chloride of density 1.594 gm/cc and Bromoform of density 2.890gm/cc were used as lower and higher density liquids respectively. The concentration of zinc atom incorporated into the doped crystals were confirmed by the EDAX spectrum. The FTIR spectrum were recorded to find the functional groups present. Powder X-ray diffraction data were collected by using an automated X-ray powder diffractometer with scintillation counter and monochromatic copper $K_\propto$ wavelength ($\lambda = 1.5406\,\AA$) radiation. The reflections were indexed following the procedures of Lipson and Steeple [12].SXRD was also taken for the pure L-Threonine crystal for comparison.

III. Results and Discussion

The photograph of all the pure and doped crystals of L-Threonine are shown in figure 1. All the crystals grown in the present study are transparent and good quality crystals. All the crystals grown in c-direction, needle shaped crystals are about 20 mm were grown.

Fig 1: Photograph of Pure and doped L-Threonine crystals

The densities of all the grown crystals are provided in table 1. The density of pure L-Threonine measured in the present study agreed with the value reported by 1.3079gm/cc [13]. The densities of doped crystals are greater than the pure L-Threonine crystal. This shows the incorporation of dopant atoms into the host lattice. EDAX spectrum shown in the Fig 2 also confirms the incorporation of Zn atoms into the host lattice.

Table 1: Values of density of pure and doped L-Threonine crystals

System	Density gm/cc
Pure L-Threonine	1.30
Doped L-Threonine	
1:0.002 Zn	1.308
1:0.004 Zn	1.362
1:0.006 Zn	1.338
1:0.008 Zn	1.380
1:0.010 Zn	1.350

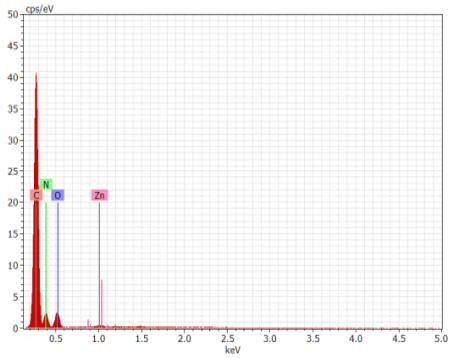

Fig 2: EDAX spectrum of doped L-Threonine 1:0.008Zn

The FTIR spectrum of pure L-Threonine crystal is shown in fig 3. FTIR spectrum were recorded for all the grown crystals in the range 4000cm^{-1} to 400 cm^{-1} . The broad band observed in the range 3169.15 and 2874.03 cm^{-1} are due to hydrogen vibration of ammonia group. The bend observed at 2048.47 cm^{-1} is assigned to nitrate . The bend observed at 1627.97cm^{-1} is assigned to asymmetric bending of NH_3 . The bend observed at 1481.38 cm^{-1} assigned to CH_2 bend. The bend observed at 1456.30 cm^{-1} is assigned to CH_3 bend. The bend observed at 1417.73 cm^{-1} is assigned to symmetric structure of CO_2 [14].The bend observed in the range 1346.36 and 1247.99 cm^{-1} are due to bending vibration of CH group. The peaks observed at 1184.33 and 1112.96 cm^{-1} is assigned to rocking of NH_3 structure . The peak observed at 1039.67 cm^{-1} is assigned to C-N stretching . The bend observed at 869.92 cm^{-1} is assigned C-C-N stretching. The peak observed at 769.62 cm^{-1} is assigned to CO_2 bending. The bend observed at 700.18 cm^{-1} is due to wagging of CO_2structure. The bend observed at 559.38cm^{-1} is assigned to rocking of CO_2. The peak observed at 489.94 cm^{-1} is assigned to torsional mode of NH_3.The bends observed at 416.64 and 443.64cm^{-1} are assigned to C-H rock.

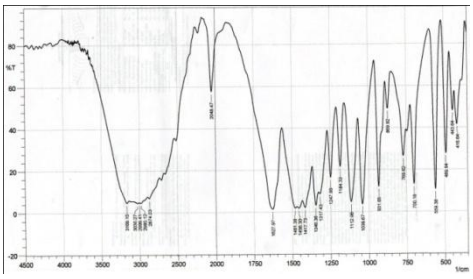

Fig 3: FTIR spectrum of pure L- threonine crystal

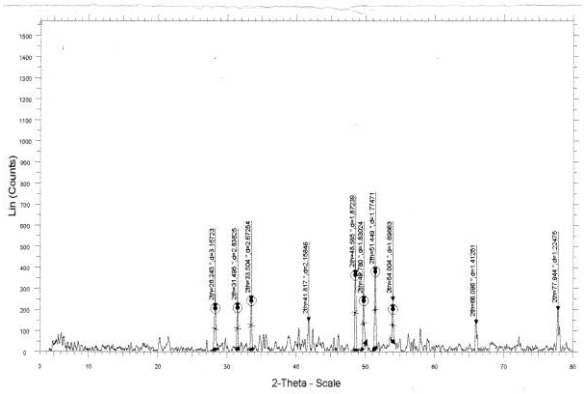

Fig 4: PXRD of 1:0.002 Zn doped L-Threonine crystal

Single crystal X-ray diffraction studies of pure LThreonine single crystal was carried out using Bruker Kappa Apex II. The crystallography data obtained from single crystal X-ray diffraction of pure L-Threonine crystal is presented in table (2). From these data, it was observed that the crystal belongs to orthorhombic system with lattice parameters a=5.140 Å, b= 7.738 Å and c=13.546 Å and a space group $P2_12_12_1$. The values obtained in the present study are closed agreement with the reported values[15].Analysis of powder X-ray diffraction data assuming the crystal structure and lattice parameters values obtained from single crystal SXRD taken in the present study, by the available methods [16].The PXRD pattern of 1:0.002 Zn doped L-Threonine crystal is shown in Fig 4. The peaks were indexed for doped L-Threonine crystal. The lattice parameters, thus calculated from the PXRD for doped crystals are also provided in table 2.From the table it is found that there is a slight variation in the lattice parameters of Zn doped L-Threonine crystals. This shows that there is a distortion in the lattice due to dopant addition

Table 2: Values of lattice parameters of pure and doped L-Threonine

System	Lattice Parameters			Volume $(Å)^3$
	a (Å)	B (Å)	C (Å)	
SXRD for Pure L-Threonine	5.140 [5.139]	7.738 [7.723]	13.546 [13.579]	538.769 [538.9] [15]
PXRD for Doped L- Threonine				
1:0.002Zn	5.042	7.784	13.680	536.928
1:0.004Zn	4.914	7.785	13.414	513.151
1:0.006Zn	4.918	7.760	14.113	538.626
1:0.008Zn	4.815	7.880	13.316	506.910
1:0.010Zn	4.941	7.748	13.556	518.977

IV. Conclusion

Crystals grown in the present study are orthorhombic in structure. The density of the doped crystals vary slightly from that of pure crystal. The incorporation of dopant atom into the host lattice is confirmed by EDAX spectrum.

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