# Growth and Structural Studies of Cu Doped L-Threonine Single Crystals

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***Abstract:*** **The Pure and Cu doped L-Threonine single crystals were grown from aqueous solution by slow evaporation technique. The density of the grown crystals was determined by floatation method and refractive index was determined by using Abbe referctometer. The grown crystals were characterized by FTIR, EDAX, SXRD and PXRD. The crystals grown in the present study, which were found to be orthorhombic, are transparent, hard and stable.**

***Keywords: L-Threonine, Crystal growth, Lattice Parameters, Density, Refractive Index, FTIR***

## I. INTRODUCTION

In view of potential applications such as optical modulation, optical switching, optical rectification, optical communication, device fabrication etc., the Non linear materials (NLO) have been a great deal of attention in research for the past two decades [1-3]. The applications of NLO materials depend upon the knowledge of material properties such as optical transparency, birefringence, thermal, electrical properties and micro hardness. The organic material L-threonine is a small naturally occurring polar and chiral amino acid and its dipole moment is nearly equal to water. Generally, Organic materials exhibit large optical susceptibilities, inherent ultrafast response times and very high Second Harmonic Generation efficiency than that of inorganic materials but they have very poor thermal and mechanical strength [4-5]. In order to enhance the mechanical hardness of the crystals, Armington et al [6] suggested two methods i) solid solution hardening ii) impurity hardening. In the present study, with intent to strengthen the organic material, the method of impurity hardening is attempted by doping the L-Threonine with the copper sulphate, an inorganic compound. Several studies on L-Threonine single crystal have been reported [7-13]. Coppe doped L-threonine was grown and characterization has been done. The results are here discussed.

## II. EXPERIMENTAL DETAILS

L-Threonine, commercially available AR grade, solvent doubly distilled water and a dopant copper sulphate ($CuSO_4$) were used to prepare the supersaturated solution in accordance with the solubility data available in the literature at an ambient temperature of $35^0$C [14]. By slow evaporation technique, the pure and Cu doped L-Threonine crystals were grown from aqueous solutions of various dopant concentration ratio Viz.1:0.002,1:0.004,1:0.006,1:0.008 and 1:0.01. One pure and five doped crystals were grown in the present study on identical conditions. The density of the six crystals was determined by floatation technique. The Carbon tetra chloride of density 1.594gm/cc and bromoform of density 2.890gm/cc were the liquids used as lower and higher densities respectively. The refractive Index of the pure and Cu doped crystals was determined by Abbe Refractometer.

The refraction energy is also calculated for the crystals. The presence of dopant Cu atoms was confirmed by EDAX spectrum and the functional groups were determined from FTIR spectrum. The Powder X-ray diffractometer (PXRD) with scintillation counter and monochromatic copper Kα wavelength (λ= 1.5406) was used to collect PXRD data for both pure and doped L-Threonine. The reflections were indexed by the procedures of Lipson and Steeple [15]. The Single Crystal X-ray diffractometer (SXRD) data were also collected for structure determination.

## III. RESULTS AND DISCUSSION

About 20mm length and needle shaped crystals were grown in c- direction. All crystals are in good quality and transparent. The photograph shows the Pure and doped L-Threonine crystals (fig.1). The densities of the crystals are tabulated in table 1. The density of pure L-threonine was perfectly matched with the literature value 1.3079gm/cc [14]. The densities of the doped crystals are greater than pure crystal. This confirms the incorporation of dopants in the host lattice. The ingestion of dopants in the host lattice was well confirmed by EDAX spectrum.

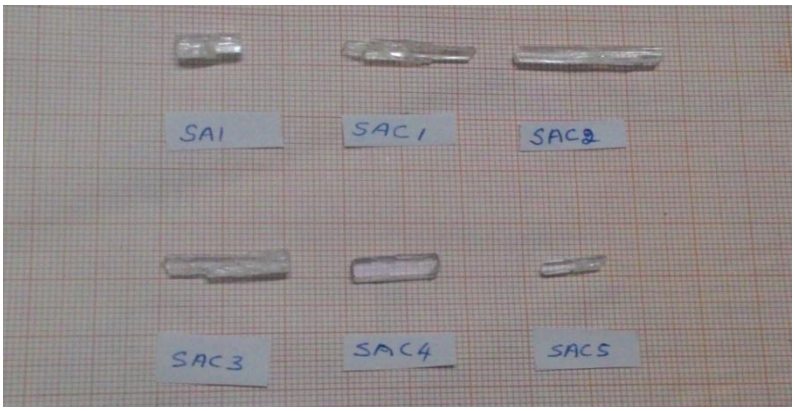


Figure 1 Photograph of Pure and Cu doped L-Threonine Crystals

Table 1: Density,Estimated dopant ratio, Refractive Energy and Refractive Index of Pure and Cu doped L-Threonine crystals

| Sample | Estimated dopant ratio | Density | Refractive Energy | Refractive index |
|---|---|---|---|---|
| **Pure L-Threonine** | **I:0.000** | **1.3** | **0.607** | **1.79** |
| **Cu doped L-Threonine** | | | | |
| **SAC1** | **I:0.001** | **1.314** | **0.63** | **1.83** |
| **SAC2** | **I:0.002** | **1.345** | **0.655** | **1.88** |
| **SAC3** | **I:0.004** | **1.445** | **0.643** | **1.93** |
| **SAC4** | **I:0.008** | **1.466** | **0.589** | **1.86** |
| **SAC5** | **I:0.01** | **1.369** | **0.651** | **1.89** |

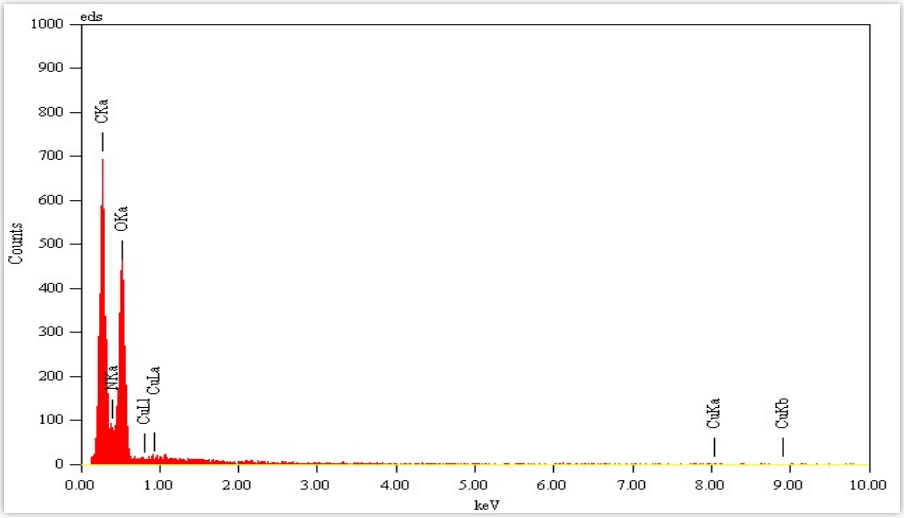


Figure 2 EDAX Spectrum of Cu doped L-Threonine 1:0.004 Cu

The FTIR spectrum of pure L-threonine is shown in fig 3. The FTIR spectrum were taken for all Cu doped L-threonine crystals in the range from 4000cm$^{-1}$ to 400cm$^{-1}$.The broad band recorded in the range 3169.15cm$^{-1}$ and 2874.03cm$^{-1}$ are ascribed to the vibration of hydrogen of ammonia group. The bend observed at 2048.47cm$^{-1}$ is due to nitrate. The bend observed at 1627.97cm$^{-1}$ is attributed to asymmetric bending of $NH_3$. The bend observed at 1481.38cm$^{-1}$ is assigned to $CH_2$. The bend observed at 1456.30cm$^{-1}$ is attached to $CH_3$. The bend observed at 1417.73cm$^{-1}$ is attributed to symmetric structure of $CO_2$ [16].The bend observed in the range 1346.36cm$^{-1}$ and 1247.99cm$^{-1}$are due to binding vibration of CH group. The peaks observed at 1184.33cm$^{-1}$ and 1112.96cm$^{-1}$are due to rocking of $NH_3$ structure. The peak observed at 1039.67cm$^{-1}$ is assigned to C-N stretching. The bend observed at 869.92cm$^{-1}$ is assigned to C-C-N stretching. The peak observed at 769.62cm$^{-1}$ is assigned to $CO_2$ bending. The bend observed at 700.18cm$^{-1}$ is due to wagging of $CO_2$ structure. 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 bend observed at 416.64 cm$^{-1}$ and 443.64cm$^{-1}$ are assigned to C-H rock.

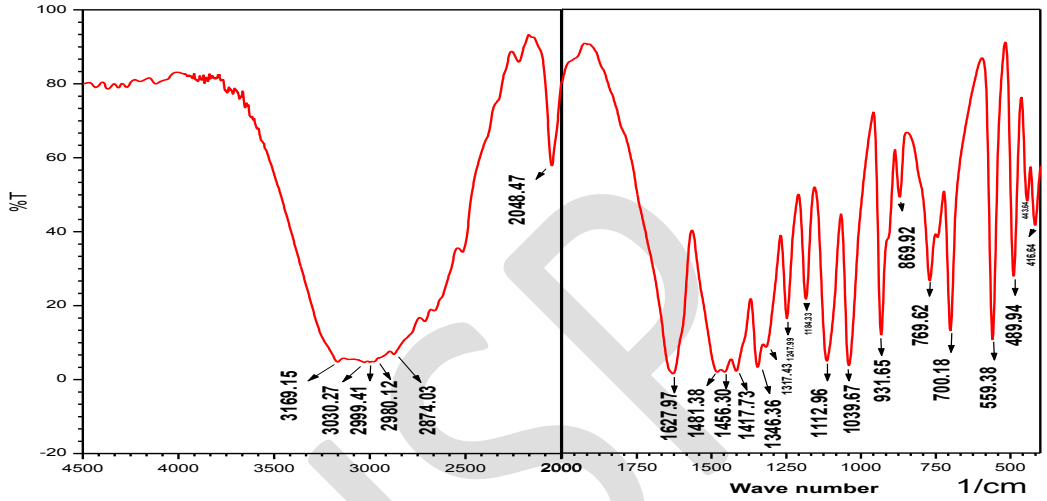


Figure 3 FTIR Spectrum of pure L-Threonine Crystal

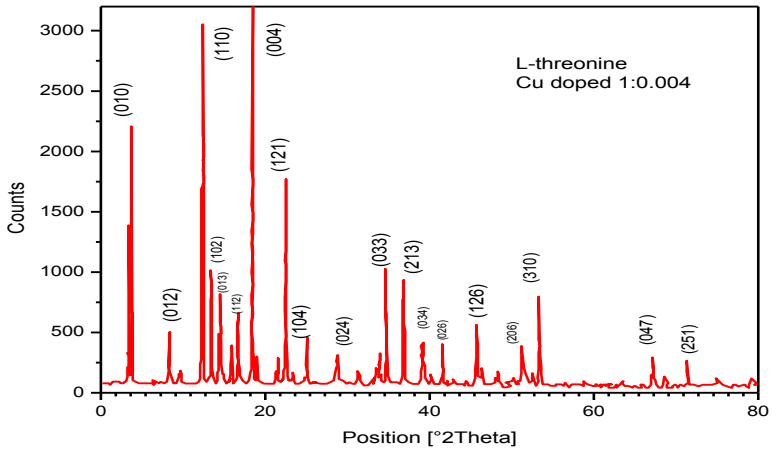


Figure 4 PXRD of 1:0.004 Cu doped L-Threonine Crystals

The powder X-ray diffraction was taken for pure and Cu doped L-Threonine crystals. The single crystal X-ray diffraction studies on L-Threonine was already carried out by using Brucker kappa Apex II.The crystallography data for pure and Cu doped L-Threonine obtained from single crystal X-ray diffraction is given in the table. The results shows that the L-threonine belongs to orthorhombic structure with lattice parameters a=5.140Å,b=7.738Å,c=13.546Å and a space group $P2_12_12_1$ as reported in the literature. The PXRD values of the lattice parameters of pure and doped L-threonine are closely matched with the standard SXRD L-threonine values [17]. The peaks were indexed for Cu doped L-threonine. The lattice parameters calculated from the PXRD for Cu doped L-threonine are provided in Table2. The table shows the slight variation in the values of lattice parameters of Cu doped L-Threonine. Hence it is evident that the addition of dopant is resulted in some distortion in the lattice parameters.

Table 2 Lattice Parameters of Pure and Cu doped L-Threonine Crystals

| **System** | **a( Å)** | **b (Å )** | **c (Å)** | **V (Å)$^3$** |
|---|---|---|---|---|
| **SXRD for Pure L-Threonine** | **5.14** | **7.738** | **13.546** | **538.769** |
| | **[5.139]** | **[7.723]** | **[13.579]** | **[538.9]** |
| | | | | **[18]** |
| **SXRD for Cu doped L-Threonine** | | | | |
| **SAC1** | **5.14** | **7.728** | **13.61** | **540.66** |
| **SAC2** | **5.118** | **7.743** | **13.615** | **539.5** |
| **SAC3** | **5.146** | **7.716** | **13.624** | **540.97** |
| **SAC4** | **5.147** | **7.735** | **13.57** | **540.26** |
| **SAC5** | **5.143** | **7.723** | **13.585** | **539.6** |
| **PXRD for Cu doped L-Threonine** | | | | |
| **SAC1** | **5.116** | **7.747** | **13.537** | **536.64** |
| **SAC2** | **5.256** | **7.333** | **13.621** | **525.07** |
| **SAC3** | **5.123** | **7.747** | **13.32** | **528.69** |
| **SAC4** | **5.141** | **7.582** | **13.579** | **535.494** |
| **SAC5** | **5.121** | **7.713** | **13.537** | **536.64** |

## IV. CONCLUSION

The grown crystals are transparent and stable. From the PXRD data, it was confirmed that the structure of the grown crystals are orthorhombic. The various functional groups were elucidated from FTIR spectrum. The presence of dopant was confirmed by EDAX spectrum. The volume of the unit cell, density and refractive index of the doped crystals nonlinearly vary with dopant concentration.

## V. ACKNOWLEDGEMENT

The Authors are indebted to the authorities of Sophisticated Analytical Instruments Facility (SAIF,Cochin)

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