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Structure and mechanical studies of L-histidine doped Tris (thiourea) Zinc Sulphate - A NLO Material

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Abstract

The tris(thiourea)zinc sulphate (ZTS) and L-histidine doped ZTS (L-HZTS) single crystals were grown by evaporation technique. The unit cell dimensions were defined by single crystal XRD. The FTIR studies validated functional groups involvement and Vickers microhardness test has defined the mechanical properties. The optical and thermal properties were identified by UV-Vis spectrometer and TG/DTA respectively. The SHG efficiency was measured using powder technique.

Keywords: single crystal, FTIR, TG/DTA and SHG.

I. Introduction

The NLO materials are developed for opto-electronic applications such as high speed information processing and frequency doubling devices have been the subject of intense research activity over the past three decades [1-3]. A continuous effort is made on the growing semi organic materials with high damage threshold and wide transparency range which make them suitable for device fabrication [4-6]. The optical and mechanical studies of L-HZTS was discussed in detail.

II. Growth and characterization

A) Synthesis of NLO Material

The ZTS was synthesized from thiourea and zinc sulphate in the ratio 3:1. The reaction as follows

$$3CS(NH_2)_2 + ZnSO_4Zn \longrightarrow [CS(NH_2)_2)]_3\,SO_4$$

The calculated thiourea and zinc sulphate was dissolved separately in distilled water. The zinc sulphate solution was transferred to the thiourea solution, ZTS salt was precipitated into the solution and then the product was separated and dried.

B) Growth of Single Crystal

The ZTS salt was dissolved in distilled water and allow for crystallization. The single crystals with a dimension of $7\times7\times3mm^3$ was grown within 25days (Fig.1). Simultaneously 1wt % of L-histidine was doped in the ZTS solution (L-HZTS) and the single crystals with of size $10\times5\times5mm^3$ were harvested in one month (Fig.2).

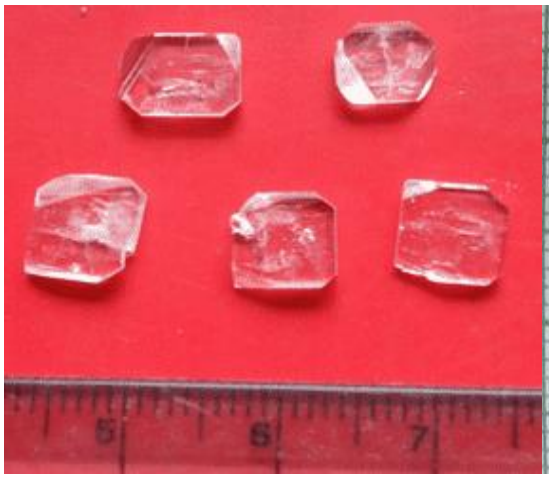

Fig.1 Grown crystals of ZTS.

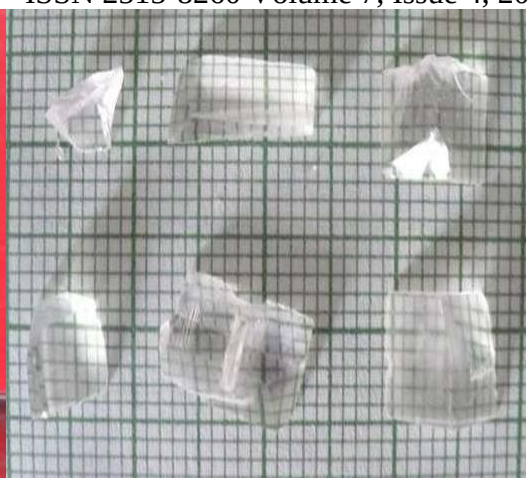

Fig.2 Grown crystal of L-HZTS.

III. Result and discussions

A) Single Crystal X-ray Diffraction

The single crystal XRDof ZTS andL-HZTS were performed using an ENRAF NONIOUS CAD-4 automatic X-ray diffractometer with MoKα radiations (λ= 0.717Å). The ZTS and L-HZTS crystal structure pertains to orthorhombic (Table 1).

Table1. Unit cell dimension of ZTS and L-HZTS.

Crystal	a(Å)	b(Å)	c(Å)	V(Å)^3	α=β=γ
ZTS	11.182	7.81	15.49	1353	90°
L-HZTS	11.11	7.7824	15.528	1342.86	90°

B) X-ray Powder Diffraction

The powder XRD of L-HZTS was carried out by D8 advance and Bruker X-ray diffractometer. Using International center for diffraction database (ICDD) software shows that red line indicates the presence of ZTS and blue line indicates the presence of L-histidine (Fig. 3).

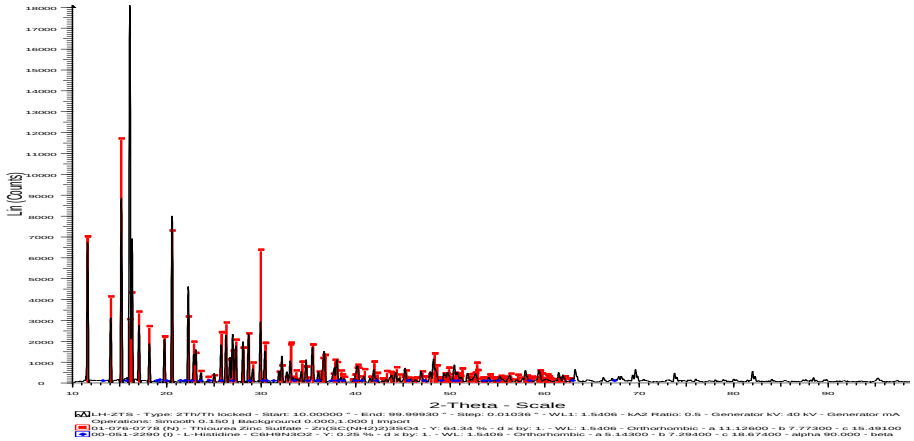

Fig. 3 Powder XRD pattern.

C) UV-Vis Spectral Studies

The UV-Vis spectrum of L-HZTS single crystal was carried out using a UV-Vis Lambda Spectrophotometer (Fig. 4). The lower cut off wavelength of L-HZTS is 270nm and the transmittance window is around 280-1100nm. Due to the dopant of L-Histidine in the ZTS solution there is absorption at 328nm has been observed.

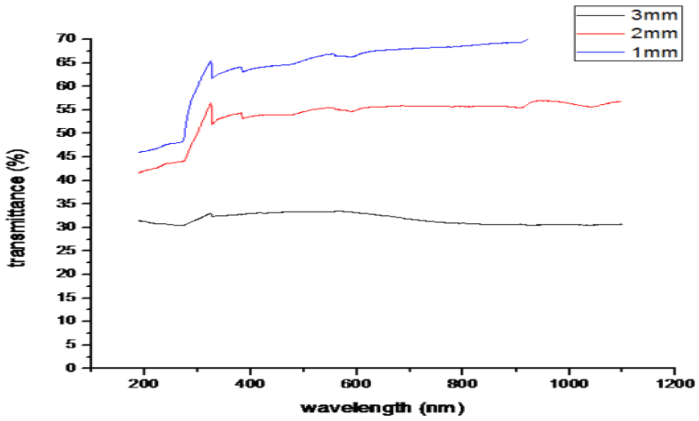

Fig. 4 UV-Vis transmittance spectrum.

D) FTIR Spectral Studies

The FTIR spectrum of L-HZTS was analyzed using KBr pellet technique (Fig.5). The peak at 1400cm^{-1} and 714cm^{-1} corresponds to the respective asymmetric and symmetric stretching vibration of C=S [5]. The vibration band at 3192cm^{-1} and 3372cm^{-1} corresponding to symmetric and asymmetric stretching of NH_2 respectively [4, 5]. The vibration band at 1511cm^{-1} and 1125cm^{-1} corresponding to stretching vibration of N-C-N and symmetric stretching vibration of C-N respectively [5]. Due to doping of L-histidine there is no shifting takes place in the ZTS crystal.

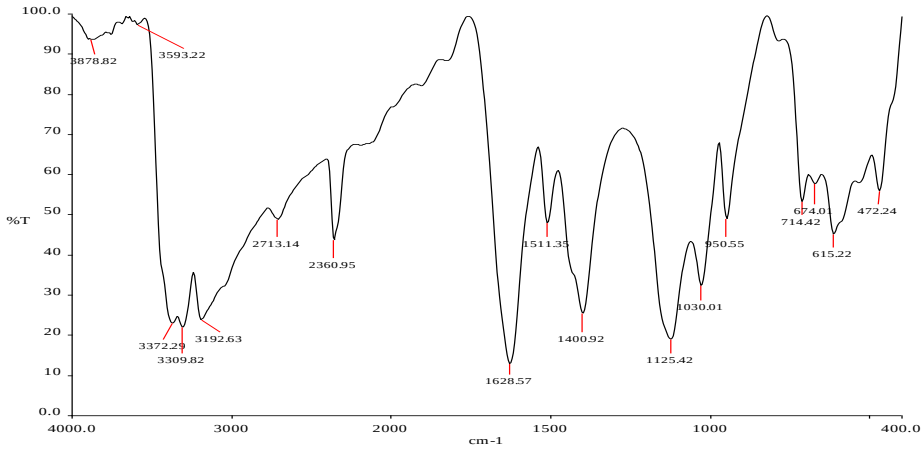

Fig. 5 FTIR spectrum.

E) Thermal Analysis

The L-HZTS thermal studies were performed using TG/DTA 6200. The TGA curve indicates that L-HZTS has good thermal stability up to 234°C and the major weight loss of 52% is between 235-320°C (Fig. 6). The melting point of L-HZTS is 235° C from DTA curve. The DSC curve shows a phase transition from solid to liquid within 235° C (Fig. 7)

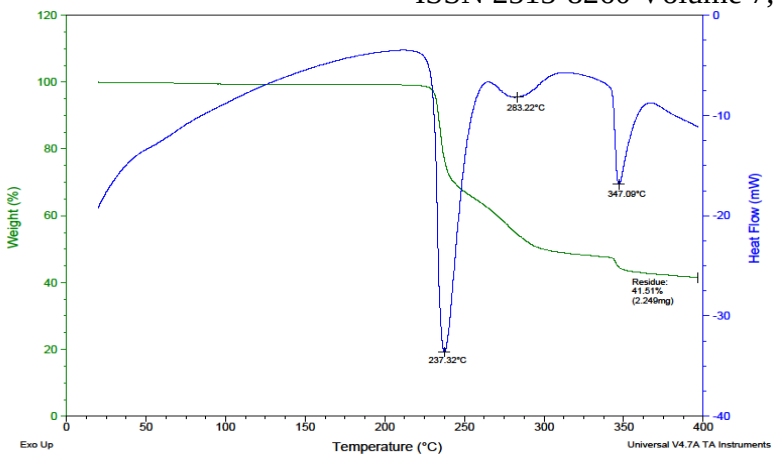

Fig. 6 TGA-DTA curve of L-HZTS.

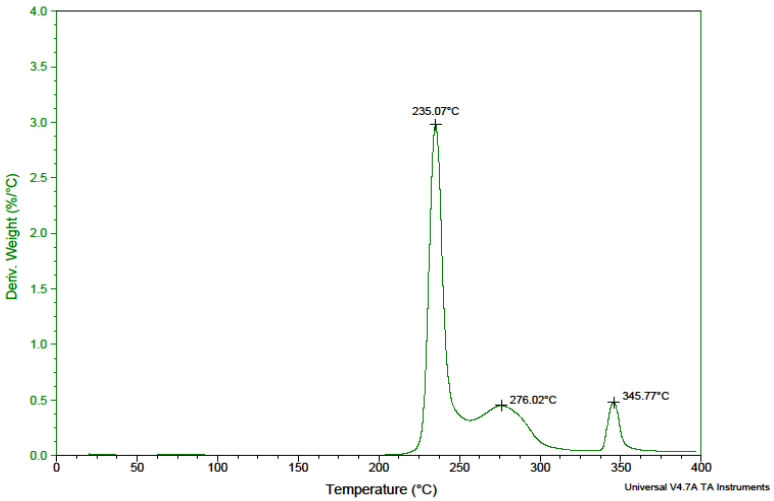

Fig. 7 DSC curve of L-HZTS.

F) Microhardness Measurement

The Microhardness measures were executed using shimadzu HMV-2 fitted with Vickers pyramidal indenter [6, 7] and the hardness increase with load (Fig. 8). The work hardening coefficient 'n' of L-HZTS was found to be 2.5 and the crystals belong to soft material category (Fig. 9).

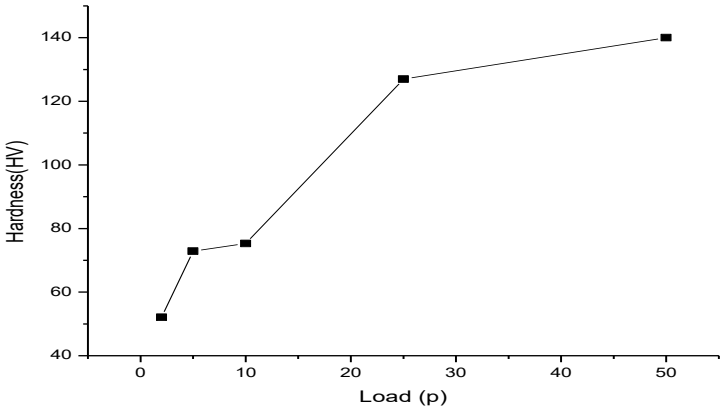

Fig. 8 Variation of hardness with load.

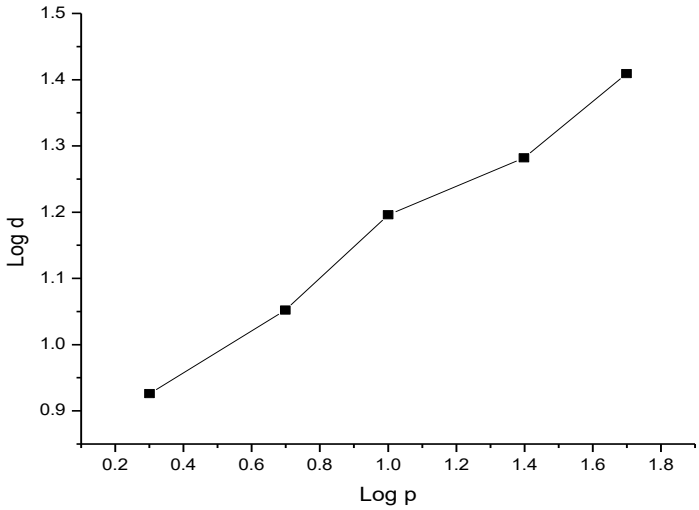

Fig. 9 Variation of Log d Vs Log P.

G) Measurement of SHG efficiency

The NLO property of L-HZTS crystal was studied by powder technique [8, 9]. The SHG efficiency of L-HZTS was 1.2 times that of KDP.

IV. Conclusion

The single crystals ZTS and L-HZTS were cultivated, and the single crystal XRD verified that both crystals belong to orthorhombic group. The powder X-ray analysis revels the presence of L-histidine was confirmed by using ICDD software. FTIR spectral analysis confirms the different functional groups and the lower cut off wavelength is 270nm. The TGA/ DTA shows good thermal stability and the L-HZTS SHG output is 1.2 times that of KDP.

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