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Structural Investigation of L-arginine doped Zinc Thiourea Acetate (ZTA) Single Crystals

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Abstract:

The structural characteristics of a single crystal of zinc Thiourea acetate (ZTA) doped with 3 and 6 mol% L-arginine are investigated in this work. Over the course of 12 days, a single ZTA crystal doped with L-arginine has formed. Zinc Thiourea acetate (ZTA), 3mol% L-arginine doped ZTA (3LAZTA), and 6mol% L-arginine doped ZTA (6LAZTA) single crystals were synthesized by the slow solvent evaporation method. Powder X-ray diffraction (PXRD) analysis verified the observed single crystals' crystalline character. Fourier Transform Infra-Red (FTIR) Spectroscopy was used to identify the functional groups present in the crystal, and the identification of the pertinent bonding peaks verified the existence of doping material.

Keywords: Crystal Growths, Structural Study, Slow Solvent Evaporation Method.

Introduction:

Numerous study domains are very interested in the Nonlinear Optical (NLO) material response that is induced in different molecules in solution and solids [1, 2]. Numerous fields, including optical communications, optical information processing, optical computing, optical disk data storage, laser fusion processes, color display, and medical diagnostics, have discovered the vast potential of NLO crystals. The prospective uses of Second Order Nonlinear Optical (SONLO) materials in developing optoelectronic technologies have garnered a lot of attention lately [3–7]. Purely inorganic NLO materials typically have excellent mechanical and thermal properties with relatively modest optical nonlinearities because of the lack of extended p-electron delocalization [8, 9]. In semi-organics, polarizable organic molecules are stoichiometrically bound with in an inorganic host. Thiourea molecules are an interesting in organic matrix modifier due to its larger dipole moment and its ability to form an extensive network of hydrogen bonds [10]. These metal–organic complexes combine the high optical nonlinearity and chemical flexibility of organics with the physical ruggedness of inorganics [11, 12]. When inorganic salt is mixed with the centrosymmetric Thiourea molecule, nonsymmetrical complexes are created that have nonlinear optical characteristics [13]. Numerous investigations into semi-organic materials doped with amino acids as possible NLO crystals have been published [14–16]. Because both organic and inorganic components directly contribute to the SHG process, the NLO characteristics of certain Thiourea complexes have garnered a lot of attention [17–19]. In order to study unique structural properties of L-Arginine doped ZTA crystal have been Synthesis.

Experimental:

Materials and Method:

The entire reagent used was of high purity and of analytical reagent (AR) grade, purchased from SD Fine. The synthesis and development of the single crystals were carried out using double-distilled water, analytic reagent grade Thiourea, zinc acetate, and L-Arginine. The ZTA crystal complex was made by dissolving Thiourea and zinc acetate in double-distilled deionized water at 2:1 mole ratios. To increase the ZTA complex's purity and decrease impurities, it underwent several recrystallizations. To dope L-arginine, a supersaturated solution of ZTA was prepared, and the carefully calculated 3 and 6 mol% of L-arginine were added gradually. The L-arginine-added ZTA solution was stirred for six hours before being filtered in a washed beaker and kept in a constant temperature bath at 38 (±0.01) ^{0}C to allow for slow evaporation. The transparent crystals were grown after the period of 12 days. To enhance the crystalline quality, the L-arginine doped ZTA crystal material underwent two progressive recrystallizations. As seen in figures 1, 2, and 3, the outcome was high-quality L-arginine-doped ZTA single crystals.

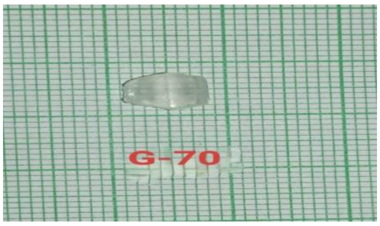

Fig 1. Pure ZTA

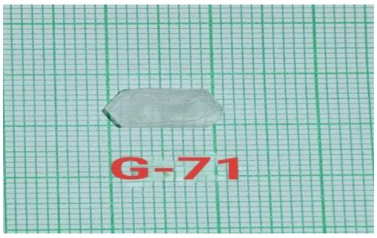

Fig. 2. 3LAZTA

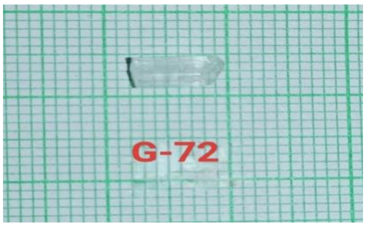

Fig. 3. 6LAZTA

Result and Discussion:

Powder X-ray diffraction (PXRD) study:

The PXRD patterns of synthesized ZTA, 3LAZTA and 6LAZTA doped ZTA single crystals is as shown in fig. 4, 5 and 6. Using the Rigaku Miniflex (II) powder X-ray diffractometer, the PXRD pattern of the ZTA and L-Arginine doped single crystals were recorded at a scan rate of 0.02 ^{o}/min in the 2θ range of 10 to 90 degrees. The observed values of cell dimensions are very well match with the reported one (Table 1). The sharp peak confirms the crystalline nature of the ZTA, 3LAZTA and 6LAZTA single crystals.

Table 1: Cell parameters of ZTA, 3LAZTA and 6LAZTA

Sr. No.	Sample	A	B	C	volume	System
1.	ZTA Reported [20]	7.1217	17.6654	11.1297	1365	Monoclinic
2.	ZTA Pure	7.0600	17.5712	10.6913	1178	Monoclinic
3.	3LAZTA	7.0564	17.5586	10.948	1174	Monoclinic
4.	6LAZTA	7.0668	17.5672	10.958	1178.8	Monoclinic

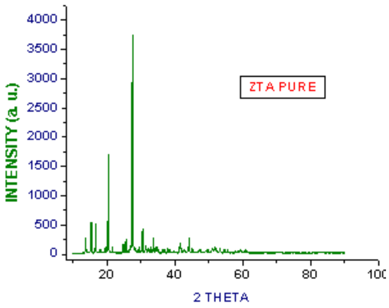

Fig 4. PXRD of ZTA

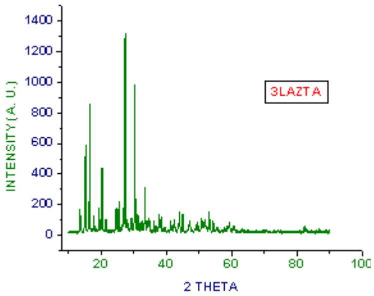

Fig. 5. PXRD of 3LAZTA

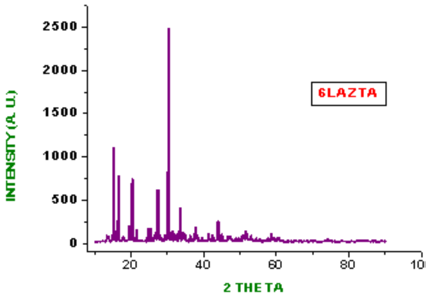

Fig. 6. PXRD of 6LAZTA

Fourier transforms infrared (FT-IR) analysis:

The FTIR spectrum of ZTA, 3LAZTA and 6LAZTA crystal is shown in Fig.7, 8 and 9. In ZTA Zinc can coordinate with Thiourea in two possible ways, i.e., through nitrogen or through sulfur of Thiourea. The high frequency N–H absorption bands in the region 3100–3400cm^{-1} is observed in IR spectra. The graph shows the various functional groups and shifting in the vibrational frequencies. Small changes of distinctive vibrational frequencies can be seen in the FT-IR spectra of both pure and doped specimens when closely examined (Table 2). Stress from dopant inclusion may be linked to the slight structural alterations that produce dispersed vibrational patterns.

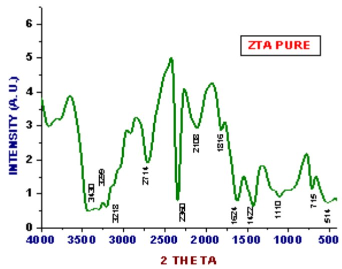

Fig 7. FTIR spectra of ZTA

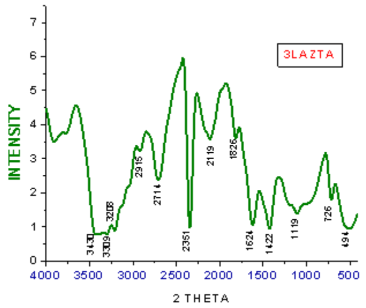

Fig. 8. FTIR spectra of 3LAZTA

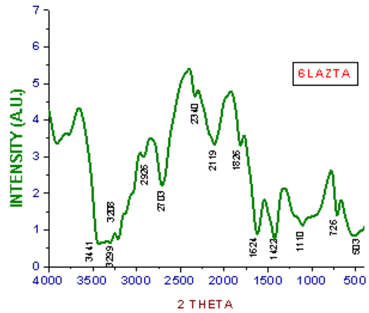

Fig. 9. FTIR spectra of 6LAZTA

Table 2. : Functional vibrations of ZTA, 3LAZTA and 6LAZTA

Sr.No.	ZTA Reported [20]	ZTA Pure	3LAZTA	6LAZTA	Assignment of Vibrations
1	3375	3430	3430	3441	NH_2 Streching vib.
2	1582	1624	1624	1624	NH_2 bending
3	1403	1422	1422	1422	C=S asym. streching
4	1135	1110	1119	1110	C=S sym. streching
5	777	715	726	726	C=S sym. streching
6	487	514	494	503	S-C-N sym. bending

Conclusion:

Single crystals of pure and L-Arginine doped Zinc Thiourea Acetate (ZTA) were grown by slow solvent evaporation method. The synthesized single crystals were transparent and can be used for further characterization. The cell parameters are very well match with the reported value. The vibrational frequency confirms the presence of different functional groups. It is evident from both XRD and FTIR studies that binding of Thiourea with zinc occurs through sulfur.

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