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To Study the Structural Properties of Cadmium Sulphate doped Tris Thiourea Zinc sulphate (ZTS) Single Crystal

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Abstract:

Slow evaporation solution growth was used to develop ZTS and Cd^{+2}-incorporated tris Thiourea Zinc sulfate (Cd-ZTS) single crystals from aqueous solution at a constant temperature. The single crystal X-ray diffraction method provided strong confirmation of the inclusion of Cd^{+2} into the crystalline lattice. The reduction in the intensities observed in powder X-ray diffraction patterns of doped specimen and slight shifts in vibrational frequencies in FT-IR indicate the lattice stress as a result of doping.

Keywords: slow evaporation, Single crystals, PXRD, FTIR

Introduction:

It is well known that the Thiourea molecule may create a network of hydrogen bonds and has a strong dipole moment. Many metal ions can combine with Thiourea molecules to create complexities of stable coordination. The coordination compounds of metal ions with a d10 electronic configuration and organic ligand Thiourea in particular have drawn a lot of interest [1-3]. These Thiourea–metal complexes can be employed as more effective substitutes for KDP crystals in laser fusion studies and frequency doubling processes. For the frequency conversion of high power lasers, zinc tris-thiourea sulphate (ZTS), also known as Zn(NH2CSNH2)3SO4, is regarded as a relatively novel and promising semiorganic nonlinear optical material. It is well known that ZTS crystal has both the mechanical and polarizable characteristics of an inorganic material. Moreover, it is shown to be less hygroscopic than KDP [4-7]. Doping ZTS crystals with inorganic or organic additions has been shown to alter their chemical and physical characteristics, which could be advantageous for device applications [8-12].

Experimental:

1. Materials:

All the reagents used were purchase from SD fine and of analytical reagent (AR) grade with high purity. Analytical reagent grade Thiourea, Zinc Sulphate and Cadmium Sulphate along with double distilled water were used for the synthesis and the growth of the single crystals. Zinc Tris-thiourea Sulphate (ZTS) salt was synthesized according to the following reaction [13, 14].

$$3CS(NH_2)_2 + ZnSO_4 \rightarrow Zn[CS(NH_2)_2]_3SO4$$

2. Synthesis Procedure:

ZTS salt was synthesized by using the 3:1 molar ratio of Thiourea and Zinc sulphate in double distilled water. The measured quantity of above salts well mixed in double distilled water using magnetic stirrer. The temperature of the stirrer should not be more than 50^0 C to avoid decomposition. To synthesis Cd^{+2} doped

ZTS single crystal 4% of cadmium sulphate is added in the solution of Thiourea zinc sulphate and stirred up to homogeneous solution. Single crystals of undoped (pure) and Cadmium sulphate-doped ZTS single crystal were grown by solution growth employing slow evaporation technique at 36^0 C temperatures. The transparent crystals were grown after the period of 10 days as shown in fig. 1 and fig. 2. The obtained crystals were collected and used for different characterization.

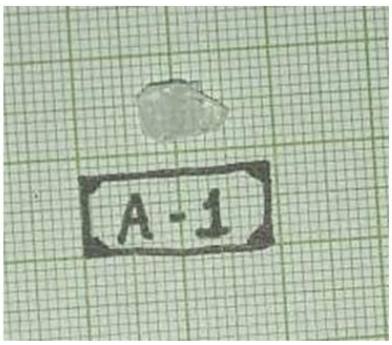

Fig.1 Pure ZTS

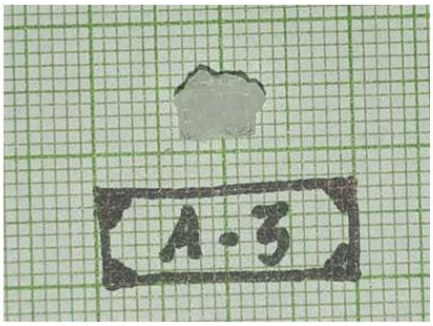

Fig. 2 Cd-ZTS

Result and Discussion:

1. Powder X-ray diffraction (PXRD) Study:

The PXRD patterns of synthesized ZTS and Cd^{+2} doped ZTS single crystals is as shown in fig. 3 and fig 4. Using the Rigaku Miniflex (II) powder X-ray diffractometer, the PXRD pattern of the ZTS and Cd-ZTS single crystals were recorded at a scan rate of 0.02 °/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 ZTS and Cd-ZTS single crystals.

Table 1: Cell parameters of ZTS and Cd-ZTS

Sr. No.	Sample	A	B	C	volume	System
1.	ZTS Reported	11.18	7.81	15.49	1345	Orthorhombic
2.	ZTS Pure	11.18	7.80	15.48	1352	Orthorhombic
3.	Cd-ZTS	11.17	7.82	15.48	1350	Orthorhombic

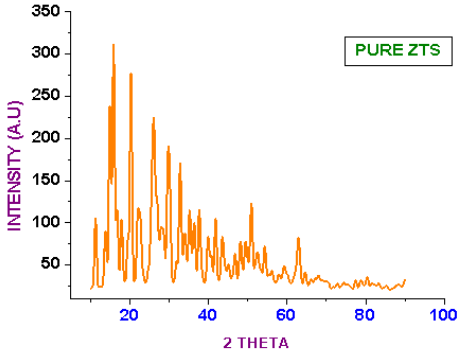

Fig. 3 PXRD pattern of ZTS

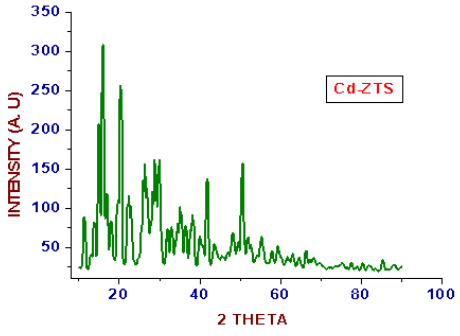

Fig. 4 PXRD pattern of Cd-ZTS

Table 2: vibrational frequencies of ZTS and Cd-ZTS

Sr. No.	ZTS Pure	Cd^{+2} doped ZTS	Assignment of Vibrations
1	3391	3380	NH_2 asym.
2	3196	3207	NH_2 sym.
3	1644	1644	NH_2 bending vibrat.
4	1438	1415	C=S asym.
5	1139	1139	C-N sym.
6	955	943	C=S sym.
7	691	702	N-C-S asym.
8	495	495	N-C-N asym.

2.Fourier transforms infrared (FT-IR) analysis:

The FTIR spectra of pure ZTS and Cd-ZTS are as shown in fig. 5 and fig. 6. 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.

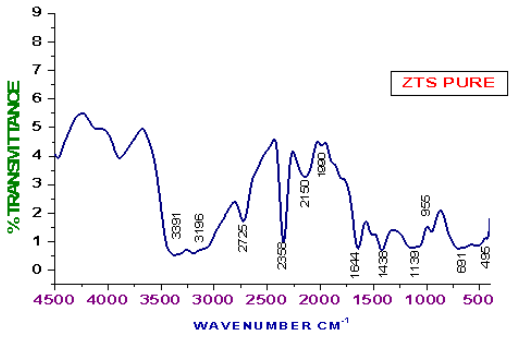

Fig. 1 PXRD pattern of ZTS

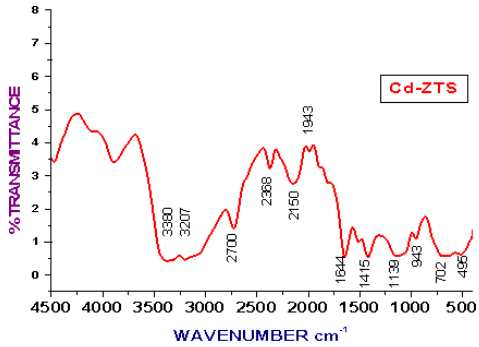

Fig. 2 PXRD pattern of Cd-ZTS

Conclusion:

Single crystals of pure and Cadmium sulphate doped Zinc Tris Thiourea Sulphate (ZTS) were grown by slow solvent evaporation method. The developed crystals had a distinct exterior look and were transparent. The pure ZTS crystals' obtained unit cell parameters match the values reported in the literature. Cd^{+2}-doped ZTS crystals have the following unit cell parameters: a=11.18 Å, b= 7.80 Å and c=15.48 Å. Through FTIR spectral analysis, the functional groups of the generated pure and Cd^{+2}-doped ZTS crystals have been determined.

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