

# Photo - Luminescence Studies of a novel NLO (ZTS) Crystal

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## ABSTRACT

Single crystals of semi organic Zinc Tris Thiourea sulphate were grown by solution growth technique. The x-ray diffraction (XRD) pattern of ZTS crystal substantiates the orthorhombic crystal structure. Temperature reliant Luminescence study from 300K to 77K (27°C to - 196°C) exhibits peaks of one violet, two blue and one green emission. Results are given and discussed.

Keywords: ZTS, photoluminescence (PL), L-Proline, Taxol.

## 1. Introduction

The Non-linear optics (NLO) receives superior brunt due to the implementation of new non-linear optical materials.

Thiourea, a centrosymmetric molecule forms non-centrosymmetric (NLO) complexes [1]. Thiourea acquires a hefty dipole moment [8, 9, 10].

The single crystals of these materials have very elevated value of laser damage threshold [3]. By considering this, the Zinc thiourea sulphate has been crystallized for the present study and characterized by the PL studies. The results have been discussed, analysed and reported.

## 2. Experimental details

The single crystals of ZTS were obtained by solution

growth technique at room temperature. The PL emission spectrum was recorded by employing 150 Watts Xe arc discharge lamp as the excitation source in the PL spectrometer.

$a=11.144\text{\AA}$ ,  $b=7.797\text{\AA}$ ,  $c=15.512\text{\AA}$ ,  $V=1348\text{\AA}^3$  and  $\alpha=\beta=\gamma=90^\circ$

with orthorhombic crystal structure of space group Pca21

and for doped ZTS with Taxol as

$a=11.152\text{\AA}$ ,  $b=7.790\text{\AA}$ ,  $c=15.518\text{\AA}$ ,  $V=1349\text{\AA}^3$  and  $\alpha=\beta=\gamma=90^\circ$ .

## 3. Results and discussions

### 3.1 PL Spectrum

The PL spectra of ZTS crystals were recorded with an excitation wavelength of 385nm for temperature ranging from 300K to 77K (for 77K, 100K, 200K, 300 K) during cooling and heating process and shown in figure 1 and figure 2 respectively[2].

Zinc gives rise to both radiative and nonradiative centres. The room temperature PL spectrum at 300K comprises outstanding violet emission peak at 409nm, sturdy blue emission at 423 nm and one very scrawny blue shoulder peak at 485 nm. Besides these, one green emission peak is identified at 527nm [4,5,6,7].

The prominent band gap violet luminescence at 409nm has shown miniature red shift with decrease of temperature from 409nm at 300K to 410nm at 77K whereas the position of all other peaks remains almost constant with respect to temperature except that of 77K as other small peak referred as shoulder peak is specified at this temperature [8, 10].

These red shifts with declining temperature go through the temperature induced band gap contraction. Therefore it is the reason to suggest that the violet emission from ZTS crystal is from Zinc vacancy related defects or their

complexes. The band gap variation is 3.02 to 3.03 eV at room temperature from the band gap luminescence by using the formula

$$E=hf$$

or

$$E=hc/\lambda$$

Where  $\nu$  is the frequency,  $\lambda$  is the wavelength of the band gap luminescence. It shows the insulating nature of the crystal nearer to the semiconducting region [11, 12, and 13].

The PL spectrum has shown ceiling emission at 409nm and ceiling absorption at 275nm respectively.

The difference between the position of the band maxima of the absorption and emission spectra of the same electronic transition [14, 15], is determined as 135nm or 9.26eV [16].

#### 4. Conclusions

Pure ZTS and doped ZTS crystals with good crystalline quality have been grown by solution growth technique. The crystals are bright, transparent and colourless with well defined emergence. The XRD study indexed the Bragg's reflections and the net crystal parameters obtained are

$$a=11.144\text{\AA}, b=7.797\text{\AA}, c=15.512\text{\AA}, V=1348\text{\AA}^3 \text{ and } \alpha=\beta=\gamma=90^\circ$$

with orthorhombic crystal structure of space group Pca21 and for doped ZTS with Taxol as

$$a=11.152\text{\AA}, b=7.790\text{\AA}, c=15.518\text{\AA}, V=1349\text{\AA}^3 \text{ and } \alpha=\beta=\gamma=90^\circ.$$

The PL spectrum shows maximum emission at 409nm which confirms the energy gap as 3.02-3.03 eV. In general the energy gap of the insulator lies above 3eV [16].

This confirms that the ZTS crystal is an insulator nearer to the semiconductor region. The nature of the crystal gives the specification whether the crystals are insulator or semiconductors. Semiconductor crystals are mostly coloured crystals and insulator crystals are transparent [9, 10, 11].

To be very patent, a crystal can have no strong electronic and vibrational transitions in the visible spectral region of 740nm to 360nm or 1.7eV to 3.5eV, generalized wavelength is 4000 - 7000 Å in the visible range.

The PL spectra collected from room temperature to 77K by cooling have shown one violet prominent emission at 409nm, one blue prominent emissions at 423nm and one very shoulder peak at 485nm and green emission peak at 527nm[12,13].

Thus the PL characteristics of doped (Taxol) ZTS crystal has been studied and reported.

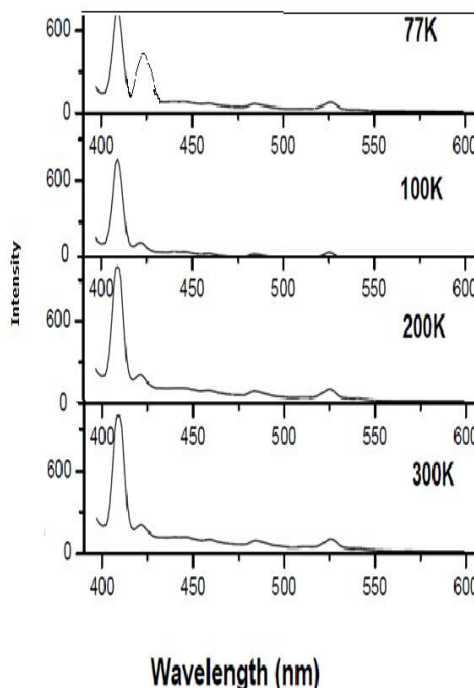


Fig 1. PL Spectra cooling process of L Proline doped ZTS

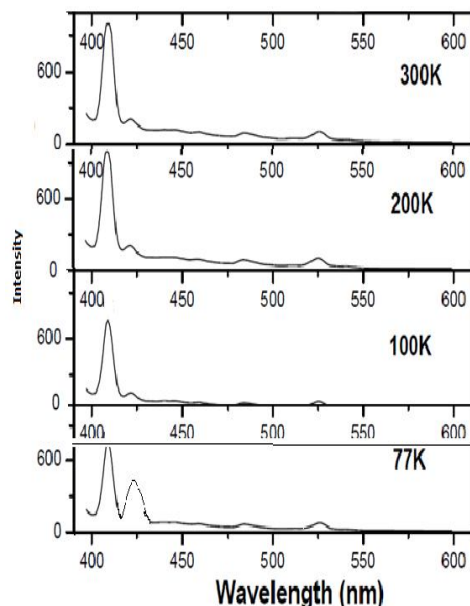


Fig 2. PL Spectra heating process of L Proline doped ZTS

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## Profile

This is K.Senthil Kannan M.Sc (Gold medalist), M.Phil, B.Ed, P.G.D.C.A., M.B.A., M.A., D.C.H., C.I., (Ph.D) and passed SLET (UGC) in the first attempt and having more than 6 years of research experience and more than one decade of academic output.

Published two books and more Papers in National and International level.



## 6. References

- [1] V.Venkatramanan, S.Maheswaran, J.N. Sherwood and H.L. Bhat, J. Crystal Growth. **179**, 605(1997).
- [2] P. M. Ushasree, R.Jeyavel, C. Subramanian and P. Ramasamy, J. Crystal Growth. **197**, 16(1999).
- [3] S.G. Bhat, and S.M. Dharmaprakash, J.Crystal Growth.**181**, 390( 1997).
- [4] G. Kanchana, D. Arivuoli, L.Kazimierz and R.Fornari, Indian J. Physics. **75A**,47(2001).
- [5] M. Dhandapani, M. A. Kandhaswamy and V. Srinivasan, Cryst. Res. Technol. **40**, 805 (2005).
- [6] [http://en.wikipedia.org/wiki/stokes\\_shift](http://en.wikipedia.org/wiki/stokes_shift).
- [7] P.Andreazza, D.Josse, F.Lefauchaux, M.C.Robert and J.Zyss, Phys. Rev. **B45**, 7640(1992).
- [8] S. Aripnammal, R. Selva vennila, S. Radhika and S.Arumugam,Cryst. Res. Technol. **40**, 896(2005).
- [9] S. Aripnammal, R.Selva vennila, S. Radhika and P. M. Ushasree, Modern Physics Letters. **B21**, 675(2007).
- [10] S. Aripnammal, S. Radhika, R. Selva vennila and N.Victor Jeya, Cryst. Res.Technol. **40**, 786 (2005).
- [11] P.M. Ushasree, Ph.D. thesis, Anna University, Chennai (1999).
- [12] P.A. Angeli Mary, S.Dhanuskodi, Cryst. Res. Technol. **36**, 1231 (2001).
- [13] B.D. Cullity, Elements of X-ray diffraction, second edition Addison Wesley Publishing Company, Inc., USA (1978).
- [14] M.M. Woolfson, An Introduction to X-ray Crystallography (Vikas Publishing House Pvt Ltd., Cambridge University Press, New Delhi 1978).
- [15] K. Swaminathan and H.M.N.H. Irving, J. Inorg. Nucl. Chem. **26**, 1291 (1964).
- [16] International Tables for X ray Crystallography

Vol IV, The Kynoch Press, Birmingham (1974).