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EFFECT OF BIS THIOUREA ZINC CHLORIDE ON OPTICAL PROPERTIES OF POTTASSIUM DIHYDROGEN PHOSPHATE (KDP) CRYSTAL

Yogesh Rasal[1], Mohd Anis[1], N.N. Shejwal[2], Mohd Azher[1], Mahendra D. Shirsat[2] and S.S.Hussaini[1*]

[1]Crystal Growth Laboratory, Department of Physics, Milliya Arts, Science and Management Science College, Beed-431122, Maharashtra, India.

[2]Intelligent Materials Research Laboratory, Department of Physics, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431004, Maharashtra, India.

*Corresponding Author, Tel.:+91 9325710500, E-mail address: shuakionline@yahoo.co.in,

ABSTRACT:

The single crystal of bisthiourea zinc chloride doped potassium dihydrogen phosphate was grown by slow evaporation solution technique. The UV-visible study was carried out using UV-Vis-NIR spectrophotometer in the range of 200-900 nm. The optical band gap of grown crystal was found to be 3.84 eV. The linear optical constants such as reflectance, refractive index and extinction coefficient were also estimated. The results of optical studies suggest that 2 mole% BTZC doped KDP crystal possesses slightly improved transparency than pure KDP.

KEYWORDS: crystal growth; optical constant; optical device

1 INTRODUCTION

Potassium dihydrogen phosphate and its isomorphs are representatives of hydrogen bonded material that posses important piezoelectric, ferroelectric, electro-optic and nonlinear properties. They have attracted the interest of many theoretical and experimental researchers probably because of their comparatively simple structure and very fascinating properties associated with a hydrogen bond system involving a large isotopic effect, broad transparency range and relatively low production cost. Improvement in the quality of KDP crystal and performance of KDP based devices can be realized with suitable dopants [1, 2]. During recent years the performance of KDP is improved with Di and Trivalent metal, rare earth elements, amino acids as dopants in appropriate percentage [3-7]. Thiourea molecule play an important role in the growth of non linear optic crystals such as bis thiourea zinc chloride, bis thiourea zinc sulphate, bismuth thiourea chloride, bis thiourea cadmium formate [8-12].

The effect of bis thiourea zinc chloride [13] and Copper thiourea complex [14] on the performance of KDP was studied. This paper reports the optical band gap and the linear optical constants of bis thiourea zinc chloride doped KDP through optical spectral analysis.

2. EXPERIMENTAL

CRYSTAL GROWTH

The 1 and 2 Mole (M) % BTZC salt were doped in the supersaturated solution of KDP and kept for slow evaporation in constant temperature bath of accuracy ±0.01 ^{0}C. Good quality transparent single crystals of 1M and 2M BZTC doped in KDP were grown within 15-20 days as shown in fig.1and fig. 2 respectively.

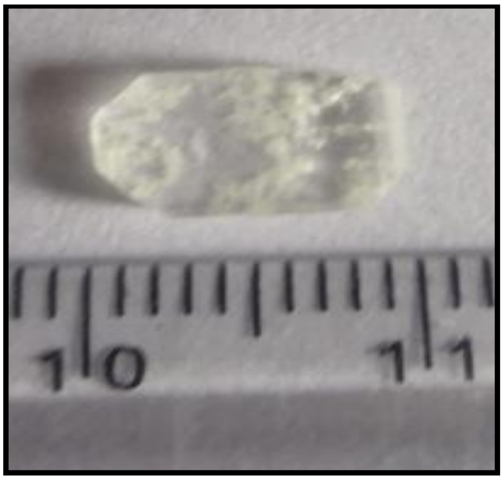

Fig.1*KDP+1M%BZTC*

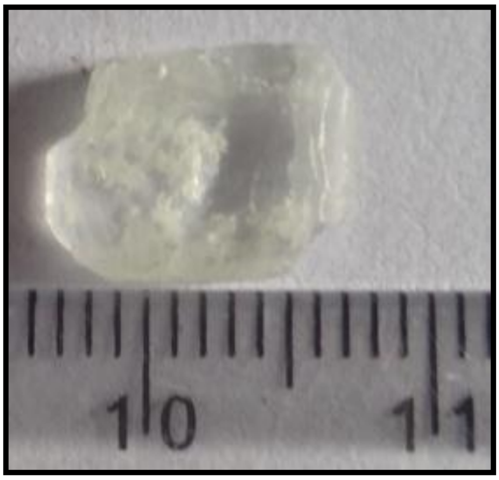

Fig. 2*KDP+2M%BZTC*

3. RESULT AND DISCUSSION

UV-VIS STUDIES

The UV-Vis studies of 1M% and 2M% BZTC doped KDP crystal was carried out using Simadzu UV-2450 spectrophotometer in the range 200nm and 900 nm. From the transmission spectrum, the 2mole% BZTC doped KDP crystal shows high transparency in entire visible region, shown in fig.3.The transmittance of 2M% BZTC doped KDP is found to be 75% in entire visible region. The values of band gap of the grown crystals were calculated from the Tauck's plot depicted in Fig. 4. The band gap is found to be 3.84 eV and 3.68eV for 1M% and 2M% BZTC doped KDP crystal respectively, indicating lower defect which is essential for fabrication of optoelectronic devices [15]. The variation of refractive index and reflectance with wavelength are shown in Fig. 5 and 6 respectivelty. The low refractive index and reflectance of doped KDP crystals in the entire UV-VIS region makes it prominent for antireflection coating in solar thermal devices and nonlinear optical applications [16]. The optical conductivity and susceptibility are shown in Fig. 7 and 8. It reveals for lower wavelengths optical conductivity and susceptibility becomes constant value. The extinction curve shows exponential decay initially and then rise up curve as shown in fig.9. The lower values of extinction coefficient $7.21*10^{-5}$ and optical dielectrics (Fig. 10 and 11) are responsible for high conversion efficiency. The comparative optical parameters of pure KDP and 1M% and 2M% BZTC doped KDP crystal are shown in table 1. The absorption coefficient was calculated by using the transmittance spectrum,

$$\alpha = \frac{2.303 \log\left[\frac{1}{T}\right]}{d} \qquad (1)$$

Where T is the transmittance, α is the absorption coefficient, d is the thickness of the crystal

Optical band gap (Eg) depicted in fig. 3 was calculated by

$$\alpha = A(h\nu - E_g)^{\frac{1}{2}} \qquad (2)$$

Extinction coefficient can be obtained by the following relation,

$$k = \frac{\alpha\lambda}{4\pi} \qquad (3)$$

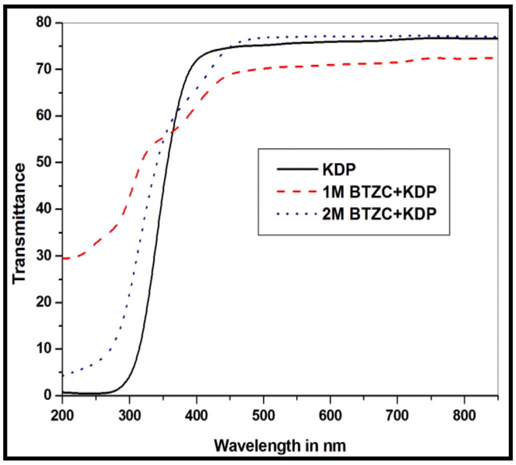

Fig. 3 *Transmittance Spectrum*

Reflectance in terms of refractive index (n) is given by relations respectively,

$$R = \frac{(n-1)^2}{(n+1)^2} \quad (4)$$

The electrical susceptibility was calculated using the relation,

$$\chi_c = n^2 - 1 \quad (5)$$

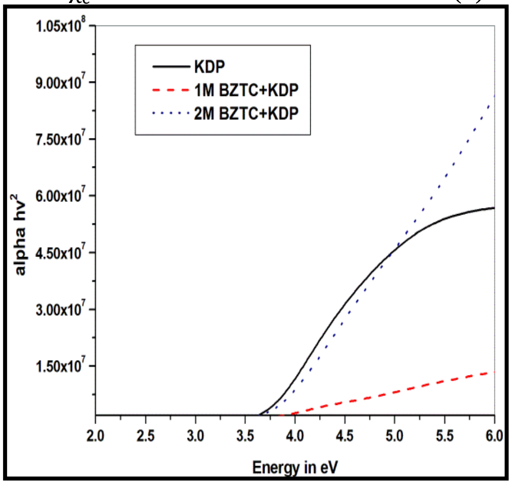

Fig. 4 *$(\alpha h\nu)^2$ vs. Photon Energy*

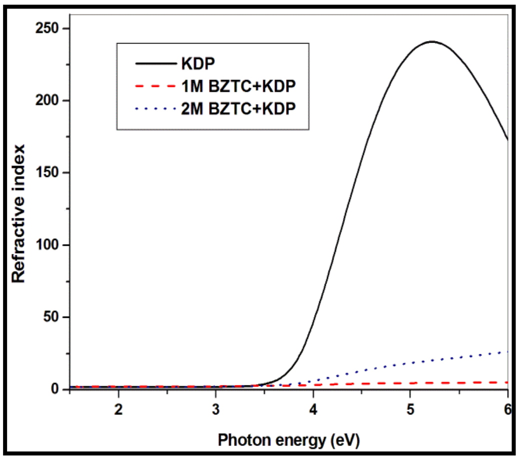

Fig. 5 *Refractive Index vs. Photon energy*

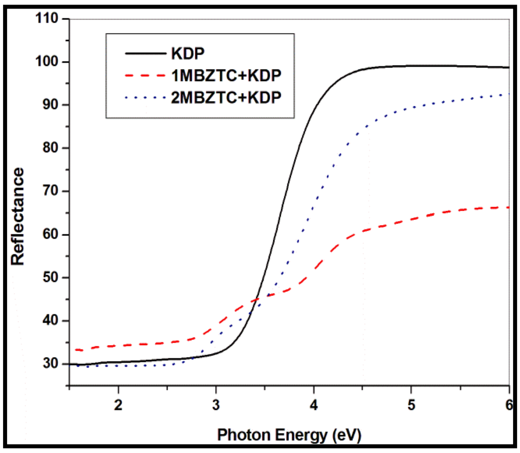

Fig. 6 *Reflectance vs. Photon energy*

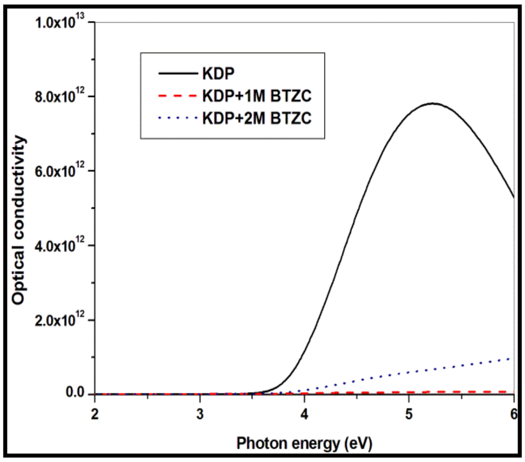

Fig. 7 *Optical conductivity vs. Photon Energy*

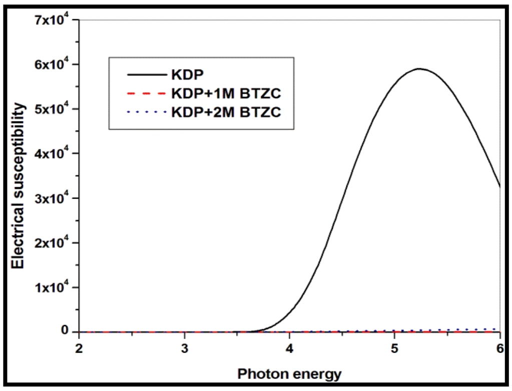

Fig. *8 Electrical susceptibility vs. Photon Energy*

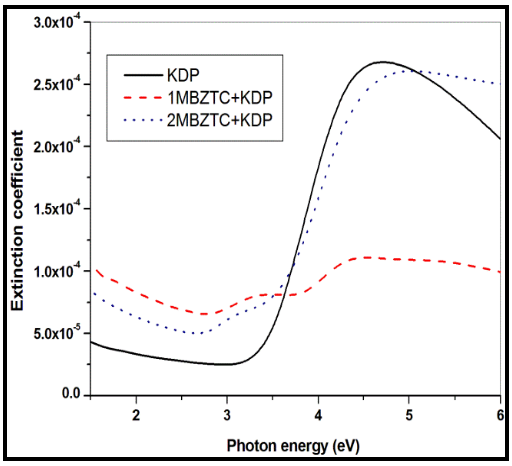

Fig. 9 *Extinction Coefficient vs. Photon energy*

Table 1 Optical parameters

Sr.No.	Physical Quantity	KDP	KDP+1MBTZC	KDP+2MBTZC
1	Band gap	3.64 eV	3.84 eV	3.68 eV
2	Cutoff wavelength	407 nm	437 nm	449 nm
3	Refractive index (at 407 nm)	1.70	1.70	1.70
4	Reflectance(at 407 nm)	32.66	39.40	37.15
5	Extinction coefficient(at 407 nm)	$2.46*10^{-6}$	$7.21*10^{-5}$	$6.42*10^{-5}$
6	Complex dielectric	4.35	4.35	4.35
7	Optical Conductivity	$2.6*10^{10}$	$2.6*10^{10}$	$2.6*10^{10}$

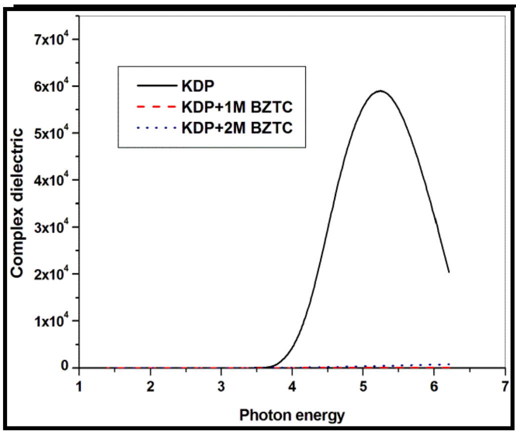

Fig. 10 *Plot of ε_r vs. Photon Energy*

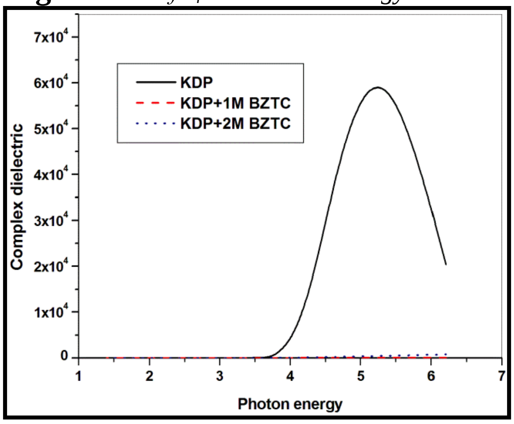

Fig. 11 *Plot of ε_i vs. Photon Energy*

4. CONCLUSIONS

BTZC doped KDP crystals were successfully grown by slow solution evaporation technique. The optical studies of grown crystal were comparatively investigated. The optical transparency of 2 mole% BTZC doped KDP crystal is higher than KDP while the large enhancement in band gap of KDP was observed with 1 mole% BTZC.The comparative study confirmed that the grown crystal may be exploited for optical device applications.

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