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ChemTech

International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN : 0974-4290
Vol.6, No.3, pp 1571-1574, May-June 2014

ICMCT-2014 [10th – 12th March 2014]
International Conference on Materials and Characterization Techniques

Growth, structural & optical Studies of Potassium dihydrogen phosphate (KDP) doped cadmium thiourea acetate (CTA) metal complex crystal

[1]R. B. Kulkarni, [2]Mohd Anis, [2]Yogesh Rasal ,
[2]S. S. Hussaini and [1]Mahendra D. Shirsat*

[1]Intelligent Materials Research Laboratory, Department of Physics, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad-431005, Maharashtra, India.
[2]Crystal Growth Laboratory, Department of Physics, Milliya College, Beed-431122, Maharashtra, India.

*Corres.author: mdshirsat_bamu@yahoo.co.in
Phone: 0919422291987, Fax: 91 – 240 – 2403113.

Abstract: In present investigation pure and KDP doped Cadmium Thiourea Acetate (CTA) crystals were grown by slow solution evaporation method at room temperature. The grown crystals were subjected to single crystal XRD to determine the volumetric parameters. The incorporation of KDP in CTA has been confirmed through the shifts in the vibrational frequencies of the grown crystals. The optical transparency of the grown crystals is examined in the range of 200- 900 nm using UV-visible studies. The transmittance data was used to determine the optical band gap and essential optical constants viz. refractive index, extinction coefficient, reflectance, electrical susceptibility of grown crystal for possible nonlinear optical (NLO) applications.
Keywords: Crystal growth; nonlinear material; Optical properties; Dielectric properties; FTIR analysis.

Introduction and Experimental

In past decade nonlinear materials has fascinated many researchers due to their vast applications in laser frequency conversion, second harmonic generations, telecommunication, electro-optic modulation [1]. CTA is the promising NLO material exhibiting better nonlinearity. The thiourea molecule can be used as an inorganic matrix modifier [2]. In literature there are reports on effect of glycine, alanine and manganese on CTA [3]. However as per the knowledge of author in literature there is no report on effect of KDP on CTA crystal. Thus in present investigation CTA is doped with KDP and grown crystal was characterized by different techniques so as to explore its possibility for NLO applications.

CTA was synthesized by dissolving calculated amount of cadmium acetate and thiourea in deionized water with 1:2 ratio according to the reaction as below,

$Cd(CH_3COO) + 2(CS(NH_2)_2)$ → $Cd(CS(NH_2)_2)_2 + 2(CH_3COO)$

The calculated ratio of 1wt% of KDP was added to the supersaturated solution of CTA and allowed to stir at constant speed for six hours to achieve the homogeneous doping throughout the solution. The optical quality crystals of CTA with the foresaid dopant were grown from saturated solution by slow evaporation at room temperature.

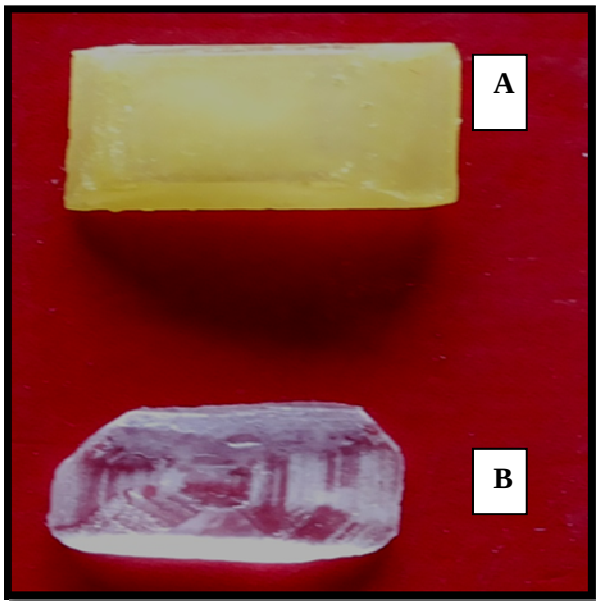

Fig.1. Pure CTA (A) and KDP doped CTA (B) crystal

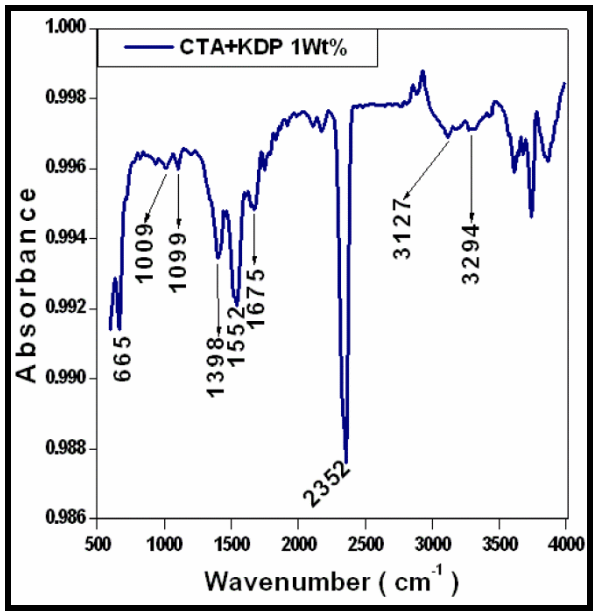

Fig.2. FT-IR spectrum of doped CTA crystal

2. Results and discussion

2.1 Single crystal XRD

The single-crystal XRD of the pure and KDP doped CTA crystals were carried using the ENRAF NONIOUS CAD4 X-ray diffractrometer. The cell parameters of doped CTA crystal are a=7.57 A^0, b=11.78 A^0, c=15.44 A^0. The analysis of XRD data revealed that the cell parameters of the grown crystals have been slightly changed with same orthorhombic symmetry of parent compound CTA [4].

2.2 FT-IR spectral analysis

The FT-IR vibrational spectrum of KDP doped CTA crystal has been recorded using Bruker ATR spectrometer in the range of 600-4000 cm-1. The identified functional groups are assigned in the spectrum shown in Fig.2 Pure CTA shows the characteristic vibrational absorption peaks at wavenumber 3431, 1667, 1495, 1398, 1110, 671 cm^{-1} [5]. The doped CTA spectrum shows NH_2 deformation peak at 3294 cm-1. The sharp peak at 2352 cm-1 is evidence of PH bond stretching of KDP. The vibrational peak of C=O bond stretching is evident at 1675 cm-1. The P-O-C bond stretching indicating the influence of KDP in CTA crystal lattice is observed at 1009 cm-1. The shifts in the vibrational frequencies of CTA crystal and prominence of PH bond stretching indicate the incorporation of KDP in CTA crystal.

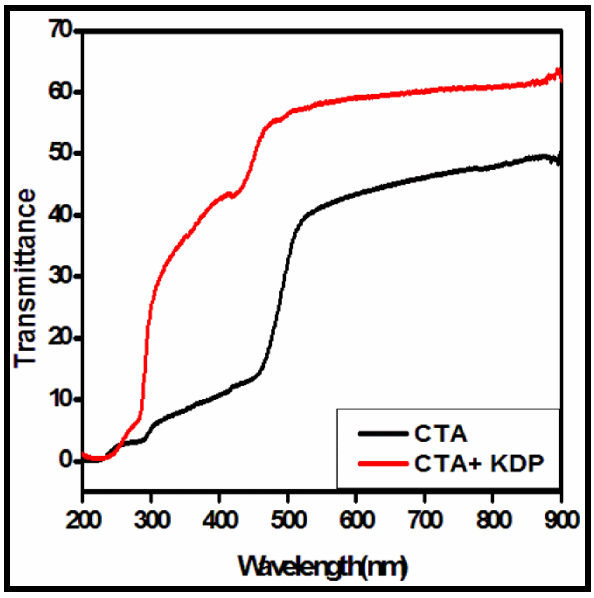

Fig.3. UV visible transmittance spectrum

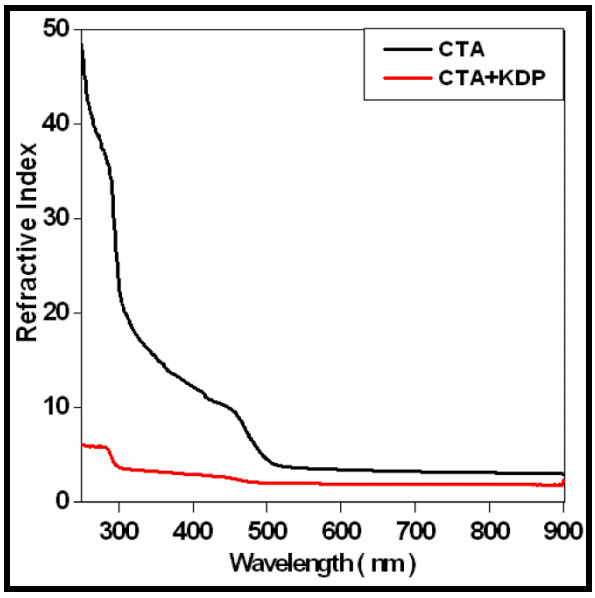

Fig. 4. Refractive index vs. wavelength

2.3 UV-visible studies

The grown crystal has been characterized by UV-visible studies using Shimadzu UV2450 spectrophotometer. The recorded transmission spectrum is shown in Fig.3. The spectrum analysis revealed that the high transparency and lower absorption edge of 416 nm has been achieved with doping of KDP in CTA crystal. The optical band gap of doped CTA crystal is depicted in Fig. 3. The optical band gap of doped crystal is determined using the taucks extrapolation method [6]. It is found to be 4.12 eV. The plot of refractive index of pure and doped CTA crystal is shown in Fig. 4. The low refractive index of doped CTA crystal vitalizes its effective suitability for determination of merit of optical reflectors, filters and resonators [7].

Conclusion

The pure and KDP doped CTA crystals have been grown by slow evaporation method at ambient temperature. The single crystal XRD confirmed the orthorhombic symmetry of doped CTA crystal with slight change in cell parameters. The shifts in the vibrational peaks of the doped CTA crystal confirmed the influence of KDP in CTA crystal. The high optical transparency and lower cut-off wavelength (416 nm) of doped CTA crystal indicates its prominence for potential NLO applications. The lower refractive index of doped CTA was also ascertained in the visible region of interest.

Acknowledgment

The authors are thankful to the University Grants Commission (UGC/41-591/2012/SR), New Delhi, and Department of Science and Technology (DST/SR/S2/LOP-22/2010), for financial assistance.

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