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Growth and Characterization of Potasium Acetate Doped BIS Thiourea Cadmium Acetate Crystals

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Abstract: ***Metal organic compounds as NLO materials have attracted much more attention for the high NLO efficiency, stable, physicochemical properties and better mechanical intention. In this work, a new semi organic mixed optical crystal of Potassium acetate doped BTCA single crystal was grown by slow evaporation method. From the powder Xray diffraction pattern, the presence of prominent peaks confirms the perfect crystalline nature. The mode of vibration of different molecular groups present in BTCA was identified by FTIR spectral analysis. The optical transparency and optical constants were assessed employing UV–visible studies.***

Keywords: Slow evaporation, Semi-organic crystal, FTIR

1. Introduction

A strong need continues to exist for NLO materials especially for lower cost, more efficient, higher average power materials in the field of optical parametric amplifier operation and second harmonic generation throughout the blue-near-UV spectral region. Much attention has been paid to metal organic compounds as nonlinear optical (NLO) materials for their high NLO efficiency, stable, physco-chemica properties [1]. The search for new and efficient NLO materials has resulted in the development of a new class of materials called semiorganics. These materials have the potential for combining the high optical nonlinearity and chemical flexibility of organic materials with the thermal stability and mechanical robustness of inorganic NLO materials [2]. Optical crystal of TZCA single crystal was grown by slow evaporation method. From the powder X-ray diffraction pattern, the presence of prominent peaks confirms the perfect crystalline nature. The mode of vibration of different molecular groups present in TZCA was identified by FTIR spectral analysis. The optical transparency and optical constants were assessed employing UV–visible studies in the range of 200–900nm.The wide optical band gap of the grown crystal has been found to be 4.09eV. Thiourea is a centro-symmetric material when it is incorporated into inorganic material. It yields excellent non-centro-symmetric material. It is also an interesting inorganic matrix modifier due to its large dipole moment. Recently researches are focusing on growing metal complexes of thiourea related crystals [3]. Metals like zinc, cadmium, mercury readily combine with thiourea resulting in stable compounds with high optical nonlinearity and good physiochemical behavior because of their closed shells [2]. Thiourea based organo metallic optical crystals like thiourea doped triglycine zinc chloride (TGZC) [4], Urea thiourea zinc chloride (UTZC), Cadmium chloride doped Zinc Tris thiourea sulphate (CZTS) [5], Halide doped Zinc Tris thiourea sulphate (HZTS) , Semi-organic Zinc Tris thiourea chloride (ZTC) [6] have gained significant attention in the last few years, because of both organic and inorganic components in them contribute specifically to the process of second harmonic generation. In the present investigation, an attempt has been made to grow a semiorganic metallic mixed optical crystal of BTCA doped with Potassium Acetate. From the powder Xray diffraction pattern the peaks which indicate the perfect crystalline structure of the material. The Fourier transform infrared (FTIR) analysis and optical transmission studies were also made.

2. Experimental

2.1 Synthesis and growth

BTCA was synthesized by mixing Analytical grade of thiourea and Cadmium Acetate (99% pure) in double distilled water in the ratio (3:1) at room temperature After preparing clear solution of thiourea, the proportional amount of Cadmium Acetate mixed gradually with continuous stirring of the solution to bring a homogenous mixture and 1 mole% Potassium Acetate was mixed as dopant. The prepared solution was filtered and allowed to evaporate slowly at room temperature. Purity of the crystal was improved by the successive recrystallization process. Good optical single crystals were harvested. The photograph of the grown single crystal is shown in Fig.1

Figure 1: Photograph of grown Potassium acetate doped BTCA Cystal

3. Characterization Techniques

3.1 X-ray powder diffraction analysis

Powder X-ray diffraction pattern was recorded for Potassium doped BTCA crystal using Rich Seifert diffractometer. When Xrays interact with a crystalline

substance, diffraction pattern is obtained. The technique is based on observing the scattered intensity when X-ray beam is incident on a sample. It is a function of the incident and scattered angle, polarization, and wavelength or energy **[6]**. The indexed pattern of the grown crystal is shown in Fig **2.**From the powder X-ray diffraction pattern, the presence of prominent Bragg's peak 2θ angle confirms the perfect crystalline structure.

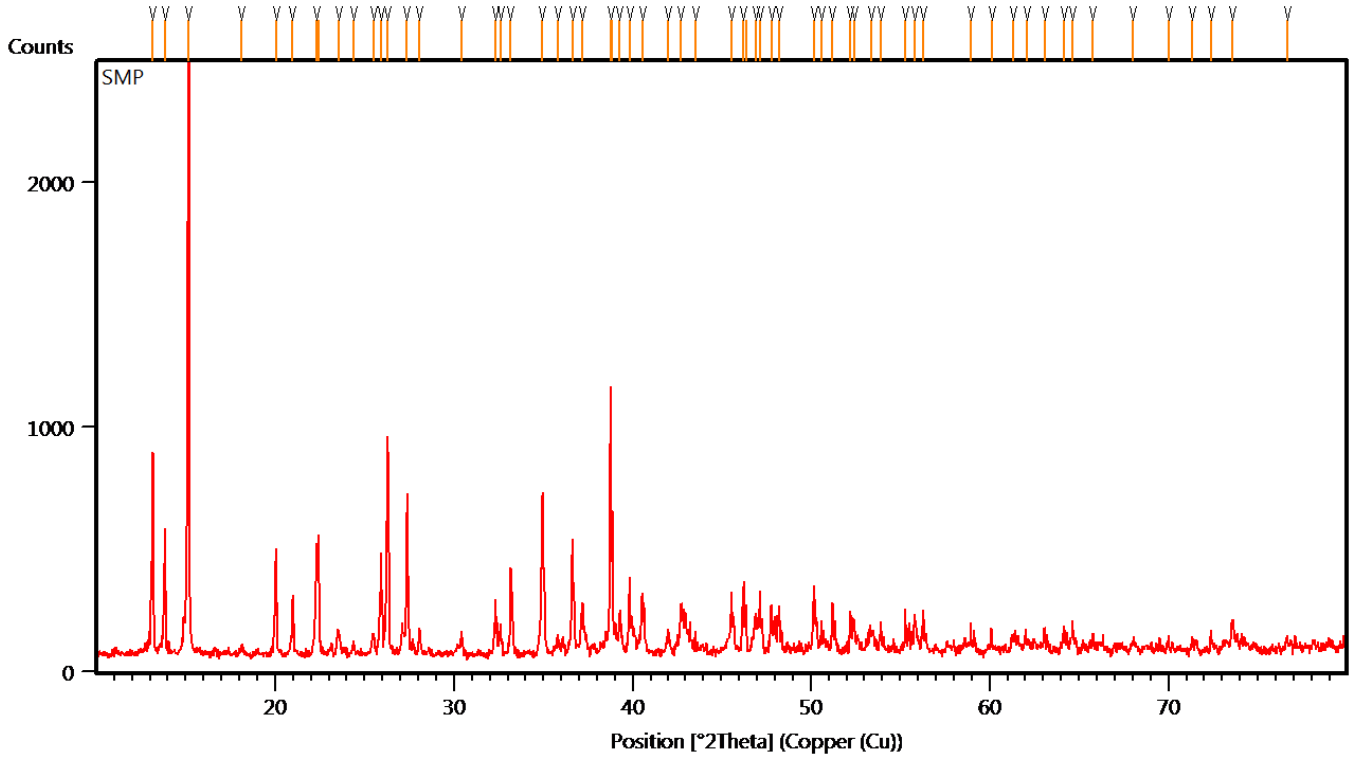

Figure 2: PXRD pattern of the grown Potassium acetate doped BTCA crystal

3.2. FT-IR analysis

The FTIR Spectrum of the grown crystal was recorded using a Bruker IFS 66V FTIR Spectrometer using KBr pellet technique in the range of 400-4000 cm-1. The vibrational measurement was carried out at room temperature.It is observed that there is a slight shifts, broadening and narrowing of absorption peaks in FTIR spectra of potassium acetate doped BTCA Crystals in the low frequency region and high transmission. This is essential for NLO property of any material **[7]** .

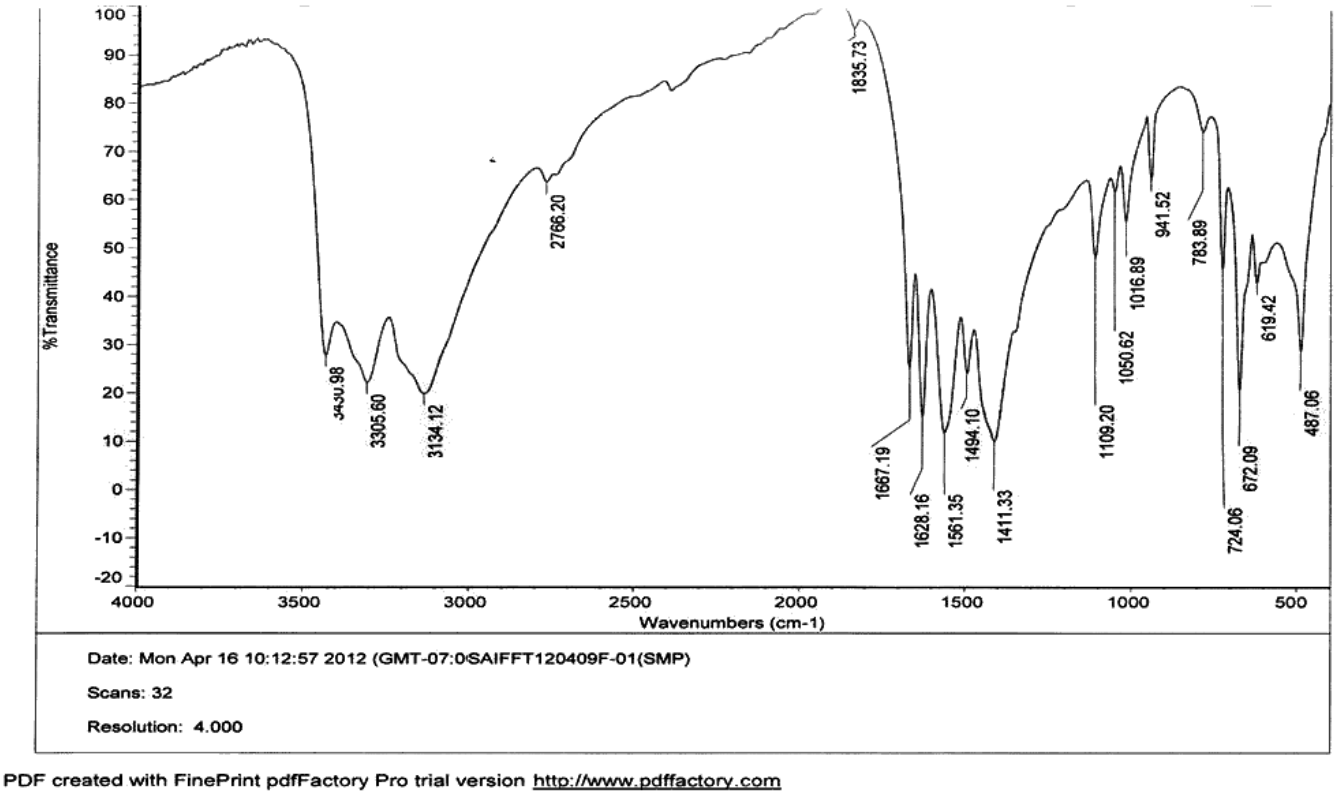

Figure 3: FT-IR Spectrum of grown crystal

3.3. UV–Visible spectral analysis

The single crystals are mainly used for optical applications. Thus the study of optical transmission range of grown crystal is important. The optical transmission spectrum was recorded using Perkin Elmer Lambda 35 spectrophotometer in the wavelength region 190– 1100 nm. The UV Vis NIR absorption spectra observed in the present study are shown in fig 4. Efficient non-linear optical crystals have an optical transparency lower cut-off wavelengths between 200-400nm. The low absorption in the visible and NIR regions along with low cut off wavelengths confirm the suitability of the grown crystals for NLO applications is an added advantage in the field of optoelectronic applications.

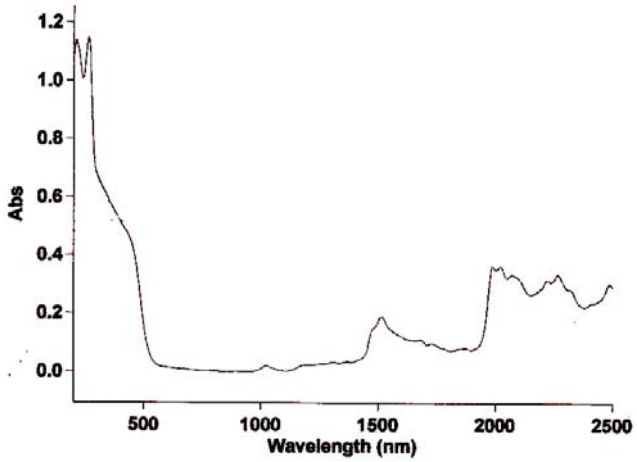

Figure 4: UV Vis NIR spectrum of grown crystal

4. Conclusion

Single crystals of Potassium acetate doped BTCA have been grown by slow evaporation technique at room temperature. PXRD shows the crystalline perfection indicate that the impurity content is minimum. FT-IR spectrum of grown thiourea crystal indicates the presence of functional groups and exhibits all the salient features. The UV-Vis spectrum shows that it has a good optical transmittance in the entire visible region and it is a potential candidate for optoelectronics application.

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