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Structural, Thermal and Optical Characterization of an Organic NLO Material – BTSCCdS

Kalokhe SB[1*], Dhumane NR[2] and Muley GG[3]

[1,2]Shri Anand College of Science, Pathardi 414102, Ahmednagar, Maharashtra, India, [3]Department of Physics, Sant Gadge Baba Amravati University, Amravati-444602,
Email: suryakantkalokhe@gmail.com

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ABSTRACT

The growth of Benzene Thiosemicarbazide Cadmium Sulphate. BTSCCdS Single crystals grown by slow evaporation growth technique, BTSCCdS crystals were grown by partial substitution of Cadmium sulphate. The incorporation of sulphate in the grown crystals was qualitatively analyzed from FTIR studies. Absoption spectra taken for the BTSCCdS crystals reveal the better Nonlinear Optical (NLO) crystal. NLO have potential uses in many devices utilizing their ability of frequency conversion, frequency mixing, electro-optic modulation etc. UV-VIS spectroscopy shows the improvement in the optical transparency. Crystal structure has been studied by powder X-Ray diffraction. Thermal analysis has also been performed on the grown crystals to study thermal stability.

Keywords: Crystal growth, BTSCCdS, FTIR, UV-VIS, EDS, Optical properties.

INTRODUCTION

In the growth of nonlinear optical (NLO) Materials there are wide applications in optoelectronic and photonic applications most of the organic crystals usually have poor mechanical and thermal properties and are susceptible for damage during processing moreover growth of bulk large size. Single crystal is difficult to grow for device application.

Inorganic materials have excellent, mechanical and thermal properties, but possess relatively modest optical nonlinearity because of the lack of extended π-electron delocalization. Due to above reasons interests have been made on semi organic crystals like higher mechanical strength, chemical stability, high damage threshold, wide transparency range which make them suitable for device fabrication. Hence it is necessary to synthesize and grow novel semi organic crystals which have positive aspects of both organic and semi organic materials.

METHODOLOGY

Benzene Thiosemicarbazide Cadmium Sulphate were taken in beaker containing doubly deionized water of 2:1 molarity. BTSCCdS crystals were grown at room temperature by slow evaporation technique by dissolving 20.84 gm of Cadmium sulphate and 0.7 thiourea in 100ml of deionized water under magnetic stirring. The temperature was maintained around 35^{o}c to avoid decomposition of element from the compound, A colorless, transparent crystal was obtained. The crystals of BTSCCdS were required up to two to three weeks for crystal formation.

Fourier transform infrared (FTIR) spectrum of BTSCCdS crystal was recorded at a resolution 2 cm-1 in the range 500 – 3500 cm-1 Employing BRUKER IFS – 66V spectrometer using KBr-pellet technique. The optical absorption and transmittance spectra of BTSCCdS crystals were recorded in the range of 200 – 1200 nm using VARIAN CARY 5E spectrometer. Energy Dispersive analysis spectra of BTSCCdS were recorded with JEOL JEO2300 Analysis Star ion of counting rate 3133cps and Energy range 0-20kev. (ZAF method Standard less Qualitative Analysis)

RESULTS AND DISCUSSION

1. FT-IR

Fourier transform infrared (FTIR) spectrum of BTSCCdS crystal shown in the Fig. 1. In the high energy region between 3470 and 2323 cm^{-1}the appearance of broad absorption band is attributed to hydrogen bond symmetric and asymmetric vibrations. The C=O group gives rise to a strong absorption in the region 1820 – 1660 cm^{-1}. The peak is often the strongest in the spectrum and of medium width. 3085 =C-H stretch for sp2. C-H occurs at values greater than 3000cm-1 (3095-3010cm^{-1}). Stretch occurs in the range 730 – 550 cm^{-1}. C-Cl stretching vibrations – These bands which appear in the range from 730 – 550 cm-1 are best observed if KBr plates or cells are used. [2] One strong C-Cl appearance in the spectrum of acetyl chloride in other aliphatic and chlorides one may observe as many as four bands due to the many confirmation that are possible. The absorption band at 1733, 1614, and 1580 cm^{-1} can be assign to C=O. the last 1580 cm^{-1} corresponds to bending of primary and secondary amides. 1505 cm^{-1} corresponds to N-O. 3085 cm^{-1}[3] Corresponds to stretch of carboxylic acid O-OH. Stretch for sp2 C-H 0ccures at values greater than 3000 cm^{-1} (3095 - 3010 cm^{-1}).

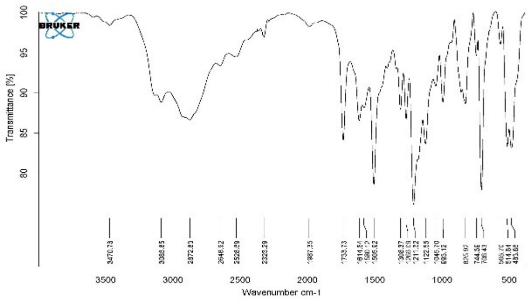

Fig. 1 FTIR Spectra

2. UV-VISIBLE SPECTRA

The optical transmission spectrum of BTSCCdS crystal was recorded in the region 200–1200 nm, using a LAMBDA 35 spectrophotometer. The recorded optical transmission spec-trum of BTSCCdS are shown in Fig. The lower cutoff wavelength of grown crystal is 190 nm. The lower cutoff wavelength of pure LSTH is 200 nm. It was observed that the CDS doped BTSC crystal had good transmittance window than pure BTSC in the region of 400–600 nm. In general the crystals had good transmittance for entire visible and IR region.[1].

3. ENERGY DISPERSIVE ANALYSIS SPECTRUM

Energy Dispersive analysis spectra of BTSCCdS were recorded with counting rate 3133cps and Energy range 0-20kev. (ZAF method Standerdless Qualitative

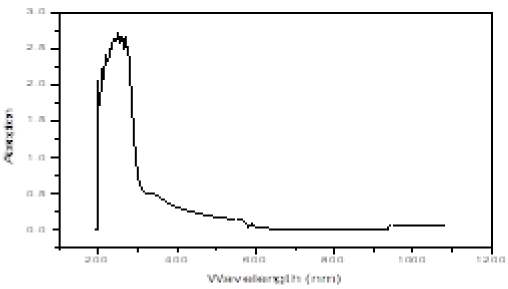

Fig. 2a. UV-visible Spectra

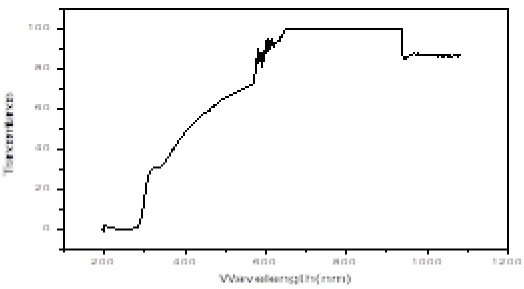

Fig. 2b UV-visible Spectra

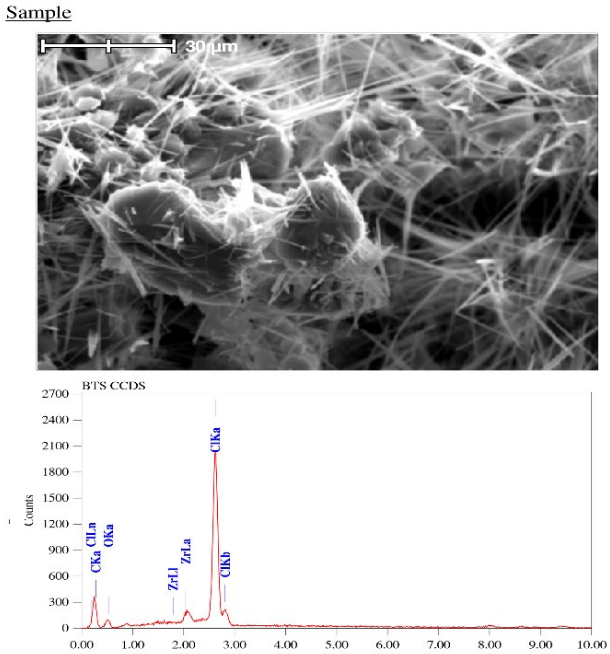

Fig. 3 EDAX Spectra

Analysis). Fig. shows the energy dispersive X-ray analysis (EDAX) of BTSCCdS. From EDAX spectrum, the presence of carbon, oxygen, zirconium and chlorine is confirmed. The incorporations of zirconium and chlorine in BTSCCdS are clearly understood from the EDAX spectral analysis[4]. The incorporation of metal ions in the sublattices may increase the number of charge carriers for the material to be dipolar.

CONCLUSION

Single crystals of CdS doped BTSC crystals have been grown by slow evaporation solution growth method. FTIR spectra confirm the presence of all functional groups present in the crystals. UV–Vis spectra show that the grown crystals of this work have good optical transmittance in the visible and IR region. The above results show CdS doped BTSC crystal is a potential material for optoelectronic applications. Microstructure and compositional analyses were discussed using EDAX studies.

Conflicts of interest: The authors stated that no conflicts of interest.

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