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Synthesis, X-Ray Diffraction, FTIR Analysis of CTSTM Crystal

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ABSTRACT
In this study, CTSTM single crystals were successfully synthesized using (NH_2 CHC=SNH_2) via the slow cooling method. The structural characterization of the synthesized crystals was carried out using X-ray diffraction (XRD) to confirm their crystalline nature. Functional group analysis and chemical composition verification were performed using Fourier Transform Infrared Spectroscopy (FTIR) and UV-Vis spectroscopy, respectively, to assess the material's optical properties. The formation of the CTSTM compound was further validated through X-ray diffractograms, with the obtained data compared against standard reference patterns from the JCPDS database. Single-crystal X-ray diffraction (SCXRD) analysis was employed to determine the unit cell parameters, providing insight into the crystal's structural arrangement. Furthermore, powder X-ray diffraction (PXRD) was conducted to identify the diffracting planes and assess the phase purity of the crystal. FTIR spectroscopy confirmed the presence of functional groups characteristic of CTSTM, while UV-Vis analysis revealed its optical absorption properties. The comprehensive characterization conclusively verifies the successful synthesis and structural integrity of CTSTM crystals, demonstrating their potential applicability in optical and electronic materials.
Keywords - CTSTM, PXRD , FTIR , UV-Vis ,JCPDS.

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I. INTRODUCTION

Most solid-state investigations depend on well-developed crystals. However, the limited availability of natural crystals or their presence in impure forms has prompted researchers to prioritize the growth of larger, high-purity, and structurally homogeneous crystals to facilitate advanced studies [1]. The selection of a material is influenced not only by the specific laser operating conditions but also by its intrinsic physicochemical properties, such as molecular nonlinearity, optical transparency, conversion efficiency, and laser damage threshold. and this study, a semi-organic material was utilized, as semi-organic compounds, [2]. which combine the advantageous properties of both organic and inorganic materials, have attracted considerable research interest. These materials exhibit high nonlinearity, a broad transparency range, and enhanced mechanical and thermal stability, making them highly suitable for advanced optical and electronic applications. [3]. This study did not include hyperfine splitting because pure powdered samples were used for characterization [4]. This research investigates the growth and characterization of nonlinear optical (NLO) single crystals, with a primary emphasis on the crystallization process. NLO materials play a crucial role in various advanced technological applications, including telecommunications, laser systems, and medical imaging, due to their exceptional optical properties. Due to the characterization of crystal, Fourier transforms infrared (FT-IR) analysis suggests the existence of water molecules and material ligands [5]. These features demonstrated potential in generating blue-violet light. Several transition metal coordination complexes, such as thiourea, thiosemicarbazide, and thiocyanate, have emerged as promising materials for NLO applications. Using a slow cooling method, the CTSTM single crystal was grown in bulk from an aqueous solution. This study systematically explores the growth of single crystals by employing diverse techniques, including solution growth, melt growth, and vapor phase growth, to optimize the crystallization process. Critical parameters influencing crystal quality—such as temperature, solvent composition, and growth rate—are meticulously analyzed to enhance optical performance. The synthesized crystals undergo comprehensive characterization through structural, functional, and optical analyses using advanced techniques.

II. MATERIALS AND METHOD

This process was conducted in a constant temperature bath, precisely maintained within ±0.01 ºC. A 300-milliliter saturated solution, prepared at 45 ºC, was filtered to remove any insoluble contaminants. For bulk growth, a seed crystal obtained through gradual evaporation was used. Prior to seeding, the solution was maintained at 45 ºC for two days. During the growth process, the temperature was gradually reduced daily at a rate of 0.01–0.2 ºC. The crystals were grown over a period of 30 to 35 days. These crystals are not only non-hygroscopic but also optically transparent.showed in fig (1).

III. FIGURES AND TABLES

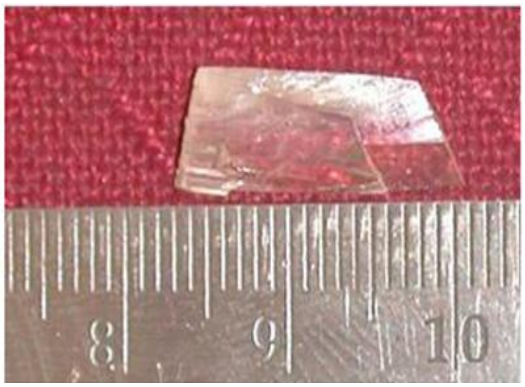

Fig 1(a) grown crystals of CTSTM by slow cooling method.

Fig 1(b): grown crystals of CTSTM by slow cooling method.

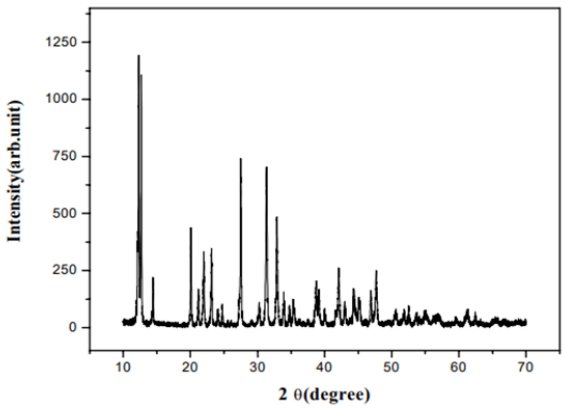

Fig 2 : Powder X-ray diffraction pattern of CTSTM single crystal.

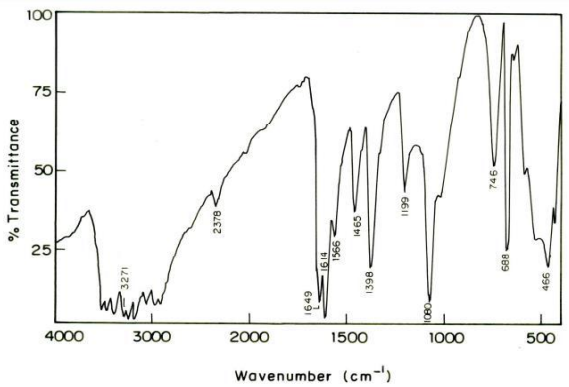

Fig 3: FTIR spectrum of CTSTM

IV. RESULTS AND DISCUSSION

The crystalline quality was further confirmed by powder X-ray diffraction analysis using X-ray diffractometer. For the single-crystal X-ray diffraction (SCXRD) analysis having dimensions of 0.2 × 0.21 × 0.33 mm³ was selected CTSTM, Cd (NH2CHC=SNH2)(SCN) a crystal with dimensions of. Intensity data were collected using MoKα radiation on a Bruker AXS diffractometer. Least-squares refinement of 25 reflections was performed within the 200–30° range. XRD analysis confirmed that the CTSTM Cd (NH2CHC=SNH2)(SCN) single crystal belongs to the monoclinic system. The estimated lattice parameters are as follows: a = 10.108 Å, b = 13.917 Å, c = 6.888 Å, and V = 968.955 Å³. These changes could include shifts in peak positions, alterations in peak intensities, or the appearance of new peaks In this pattern, diffraction peaks are observed at specific angles, corresponding to the atomic spacing within the crystalline lattice of the material [6].shown in fig (2).

FTIR analysis of powdered CTSTM confirmed functional groups and ligand coordination. The spectrum (4000–450 cm^{-1}) was recorded using the KBr pellet method on a Perkin

Elmer infrared spectrometer. A broad band (2100–3500 cm^{-1}) and a sharp peak at 3271 cm^{-1} indicated O–H (H_2O) vibrations. NH_3^+ hydrogen bonding was evident in the low-energy region. Peaks at 1649 and 1614 cm^{-1} corresponded to Q(C=S), with 1649 cm^{-1} linked to NH_3^+ bending. Metal coordination was confirmed by a shift to 1614 cm^{-1}. The absence of Q(NH_2) at 2063 cm^{-1} indicated amino-nitrogen coordination. Q(N–N) vibrations appeared at 1001 cm^{-1}, resistant to red shift at 1080 cm^{-1}. Thiosemicarbazide absorption bands were noted near 1610, 1379, 1199, and 1080 cm^{-1}[7].FTIR analysis predicts the presence of functional groups and cadmium integration into the material's sublattices. Cadmium ions significantly enhance the material's polarizing capacity [8][9][10].Showed in fig (3).

V. CONCLUSION

i] A single crystal XRD analysis was conducted to evaluate the lattice parameters. X-ray diffraction measurements confirmed that the resulting crystal exhibits a monoclinic orientation.

ii] FTIR analysis confirms the presence of functional groups and the successful integration of cadmium into the material's sublattices. The incorporation of cadmium ions notably improves the material's polarizing capacity.

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