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Original research article

Influence of L-lysine on optical and dielectric traits of cadmium thiourea acetate complex crystal

Imran Khan[a], Mohd Anis[b], Umar Bhati[c,*]

[a] Almahmood International School and Junior College of Science, Akola, 444006, Maharashtra, India
[b] Department of Physics, Sant Gadge Baba Amravati University, Amravati, 444602, Maharashtra, India
[c] Department of Physics, Shri Shivaji Arts, Commerce and Science College, Akot, 444101, Maharashtra, India

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ABSTRACT

Crystals enduring strong thiourea-metal coordinated ligand demonstrate outstanding combination of dielectric and optical properties which are exclusively desirable for nonlinear optical (NLO) device applications and thus current study has been designed to investigate the semiorganic cadmium thiourea acetate (CTA) complex crystal. The pure and L-lysine (LL) influenced CTA complex crystals have been grown by commercial slow solvent evaporation technique at room temperature. The structural parameters of grown crystals have been experimentally determined by means of single crystal X-ray diffraction technique. The UV–vis spectral analysis has been employed within the wavelength range of 200–1100 nm to examine the effect of LL on optical transparency and extinction coefficient of CTA crystal. The enhancing effect of organic ligand of LL on second harmonic generation (SHG) efficiency of CTA complex crystal has been discussed and the SHG efficiency has been determined by employing the Kurtz-Perry powder test. The reliance of dielectric constant and dielectric loss of pure and LL influenced CTA crystal on temperature has been examined within the range of 35–90 °C. The compatibility of LL doped CTA crystal for distinct technological device applications have been explored.

1. Introduction

Since past many decades semiorganic nonlinear optical (NLO) thiourea metal complex crystals have been introduced to the scientific fraternity as an interesting material owing to their ability to inherit good structural, optical, physical, mechanical and thermal properties. Certainly the NLO crystal with such large diversity of appealing characteristics can be readily subjected to optoelectronics, photonics, frequency conversion and optical communication device applications [1–4]. The large variety of thiourea metal complex crystals have been designed, grown and investigated in later past [5]. It is attention grabbing fact that the transition metals (Zn and Cd) having d^{10} shell electrons favor excellent optical properties [6] hence out of the vast family of thiourea metal complex crystals the cadmium thiourea acetate (CTA) complex crystal holds strong research impetus. The fundamental properties of CTA crystal has been studied by several research groups by employing conventional and unidirectional growth techniques [7–10]. It is acknowledged that presence of additive effectively decorates the properties of host crystal [11,12], hence further progress in uplifting the properties of CTA crystal has been achieved by doping different organic and inorganic additives by many researchers. The influence of glycine, L-alanine and Mn^{2+} on properties of CTA crystal has been explored [13]. Recently our group comparatively investigated the impact of amino acid L-valine, L-cysteine and L-threonine on UV–vis, third order nonlinear optical and dielectric

* Corresponding author.
E-mail address: umarbhati2008@rediffmail.com (U. Bhati).

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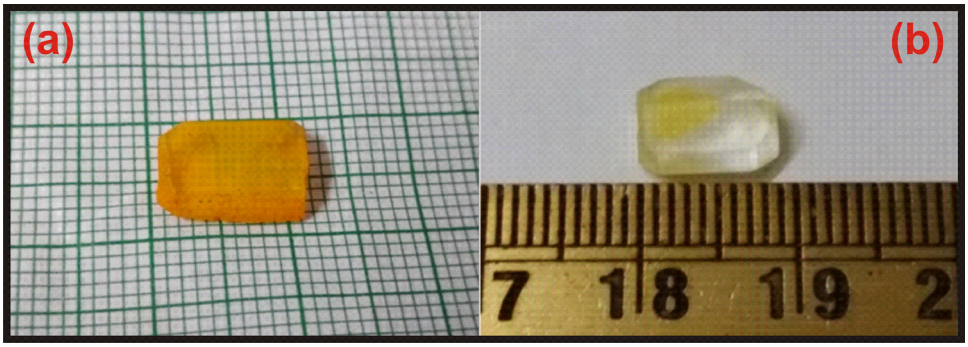

Fig. 1. Single crystal of (a) CTA and (b) LL-CTA.

properties of CTA crystal [14–16]. The literature analysis reveals that the amino acids possesses Zwitter ions, wide H-bonding network, chiral centers and carboxyl group with abundance of pi bond [17] which are essential for tailoring the characteristic properties of host crystal and thus clarifies their importance for optimizing the properties of CTA crystal. In current investigation we propose the addition of chiral amino acid L-lysine (LL) in order to improve the overall performance of CTA crystal. The studies have been accomplished by employing different characterization techniques which include the single crystal X-ray diffraction, UV–vis, Kurtz-Perry test and dielectric analysis.

2. Experimental procedure

The Merck make AR grade cadmium acetate and thiourea was measured in 1:2 mol ratio as starting material and respectively dissolved in deionized water. This solution was allowed to stir and the cadmium thiourea acetate (CTA) complex was synthesized by slow solvent evaporation method. Further the saturated solution of CTA complex was prepared and 0.5 mol of L-lysine (LL) was gradually added and allowed to stir for five hours in order to facilitate the homogeneous mixing of LL. This LL influenced CTA (LL-CTA) solution was then filtered in clean rinsed beaker using the Whatman filter paper. The beaker containing the filtrate of LL-CTA solution was housed in the constant temperature water bath maintained at 36 °C. As the pure and LL-CTA solution progresses the process of slow evaporation the crystals were harvested within period of 3 weeks. The pure and LL-CTA crystal is shown in Fig. 1a and b respectively. It is noticeable that LL-CTA crystal express superior optical quality and morphology as compared to CTA crystal which confirms the constructive involvement of LL in optimization.

3. Results and discussion

3.1. Single crystal X-ray diffraction (XRD) analysis

The grown pure and LL-CTA single crystals were subjected to XRD analysis using the X-ray diffractometer (Model: Enraf Nonius CAD4). The crystallographic data of grown crystals have been experimentally determined at room temperature and systematically tabulated in Table 1. It is observed that the pure and LL-CTA crystal express orthorhombic crystal symmetry belonging to the space group $P2_12_12_1$. It is noteworthy that there is marginal difference in unit cell dimensions of pure and LL-CTA crystal which might have been expressed due to essential impact of LL on lattice site of host crystal CTA. The incorporation of LL however did not alter the structure and space group of CTA crystal.

3.2. Optical studies

The linear optical properties (transmittance and extinction coefficient) of pure and LL-CTA crystal has been evaluated within the wavelength range of 200–1100 nm using the spectrophotometer (Model: Shimadzu UV-1601). The optical transmittance in a crystal is attributed by permitted electron transitions, materials composition, molecular anisotropy and the defects (structural and crystalline)

Table 1
Single crystal XRD data.

Structural parameter	CTA	LL-CTA
a (Å)	7.56	7.58
b (Å)	11.79	11.94
c (Å)	15.82	15.99
V $(Å)^3$	1410.07	1447.17
Crystal system	Orthorhombic	Orthorhombic
Space group	P_{212121}	P_{212121}