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Growth and characterization of Tetra-thiourea strontium chloride crystals

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Abstract

There are various nonlinear optical materials having crystalline nature and find various applications in science and technology. Tetra-thiourea strontium chloride was synthesized and single crystals were grown by the slow solvent evaporation technique using aqueous solvent. The grown crystals were characterized by Fourier Transform Infrared Spectroscopy (FT-IR), and X-ray diffraction analysis (XRD). The FT-IR spectra of these crystals were recorded in the wave number range 400-4000 cm^{-1} which reveals the presence of various functional groups. The powder XRD analysis suggested orthorhombic crystal structure.

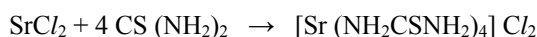
Keywords: Tetra-thiourea strontium chloride, FT-IR, XRD.

1. Introduction

Nonlinear Optical (NLO) materials crystals are of considerable interest and of great demand because of their different applications in science and technology, such as different harmonic generators, sum and different generators and parametric oscillators [1-2]. The inorganic and organic class of NLO materials is also available with different merits and demerits [3-4]. The semi-organic class of NLO materials possesses both the properties of organic and inorganic NLO materials [5-7]. Metal complexes of urea and urea analogs have been explored [7]. Bis-thiourea cadmium chloride [8] and bis-thiourea zinc chloride [9] crystals have been synthesized, grown and characterized, which exhibit good NLO properties. Compared to other similar crystals, bis-thiourea cadmium chloride exhibit more laser induced damage threshold values [10]. Recently, tetrakis thiourea nickel chloride [11], bis-thiourea bismuth chloride [12] and zinc tris thiourea sulphate [13] crystals are reported which are urea based semi-organic NLO crystals. In the present study we have synthesized tetra-thiourea strontium chloride (TTSC) crystals by slow solvent evaporation method. The grown crystals were characterized by FT-IR and powder XRD.

2. Experimental

The slow solvent evaporation method was used to synthesize TTSC crystals. AR grade thiourea and strontium chloride was used in double distilled water. The expected chemical reaction was



The synthesized salt was purified by several time re-crystallizations. TTSC single crystals were grown by slow evaporation technique at room temperature. The growth vessel was closed and through a small opening slow evaporation was allowed. A constant temperature water bath with ± 0.1 °C accuracy was used to maintain the constant temperature. Crystal growth was completed in about 10 days. In the present investigation, the growth of TTSC single crystals by slow evaporation technique at room temperature and its characterization by using FT-IR and powder XRD are reported.

3. Result and Discussion

FT-IR study

The FT-IR spectrum of bis-thiourea zinc chloride [14], zinc tris thiourea sulphate [15], bis-thiourea strontium chloride [17] and tris-thiourea strontium chloride [18] have been reported.

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The FT-IR spectrum of the grown crystals was recorded in the wave number range 4000-400 cm^{-1} . Figure 1 shows the spectrum of the grown crystals.

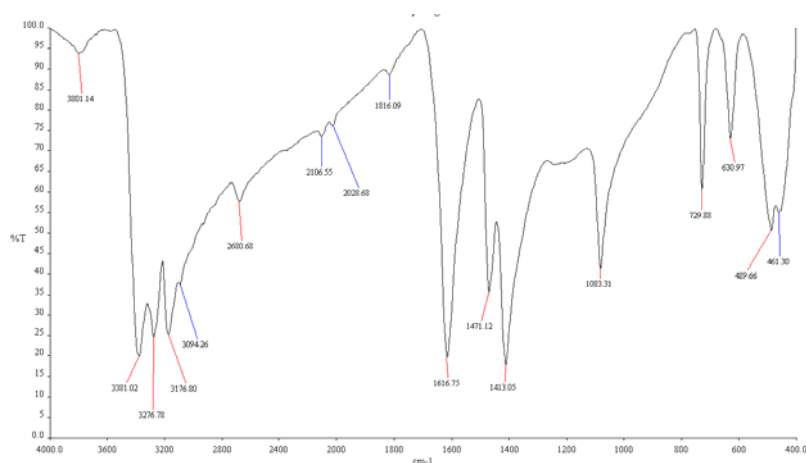


Fig 1.

The C – S stretching vibrations occur at 3276 cm^{-1} , while the C – S bending occurs at 1083 cm^{-1} . The N – H primary stretching vibrations occur at 3381 cm^{-1} and 3176 cm^{-1} , while the NH_2 stretching vibrations occur at 1471 cm^{-1} . The vibrations occurring below 900 cm^{-1} may be due to metal and halogen bonding vibrations.

Powder XRD study

The XRD of bis-thiourea strontium chloride [17] and tris-thiourea strontium chloride [18] have been reported. The grown crystals have been characterized by powder X-ray diffractometer. Figure 2 represents the powder X-ray pattern of grown crystals.

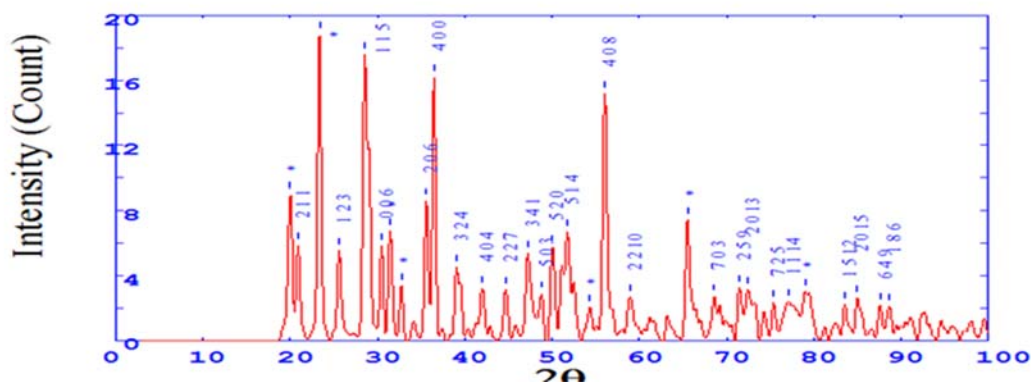


Fig 2.

Using powder X computer software the h , k and l parameters as well as d and 2θ values were generated in such a way that these values match with the powder X-ray diffraction pattern. The estimated values of unit cell parameters of TTSC crystals are $a = 9.850 \text{ \AA}$, $b = 9.600 \text{ \AA}$, $c = 17.600 \text{ \AA}$ and $\alpha = \beta = \gamma = 90^\circ$, which shows orthorhombic crystal structure. Earlier workers reported the powder XRD study and estimated the unit cell parameters of bis-thiourea zinc chloride [14]. Orthorhombic form of BTCA was also reported earlier [16].

4. Conclusion

TTSC crystals were grown by slow solvent evaporation technique. The grown crystals were characterized by FT-IR spectroscopic and XRD. The FT-IR spectrum of the grown crystals revealed the presence of C – S and N – H bond. From the XRD study of the grown crystal, the estimated values of unit cell parameters of TTSC crystals were found

to be $a = 9.850 \text{ \AA}$, $b = 9.600 \text{ \AA}$, $c = 17.600 \text{ \AA}$ and $\alpha = \beta = \gamma = 90^\circ$, which confirmed the orthorhombic crystal structure.

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