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Analysis of Non-Linear Characterization for Optical Properties of Thiourea Tartarate

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Abstract:

In recent years, Analysis of nonlinear optical characterization of Crystals play an important role in the opto-electronics and frequency conversion device applications. The preset work aim to synthesis and grow Thiourea tartrate single crystals by slow evaporation solution growth technique for higher Non Linear Optical efficiency. Thiourea Tartrate single crystals have been grown by the slow evaporation method at room temperature using aqueous solution. The prepared crystal structural characterization, Thermal stability, Impedance properties and NLO studies were carried out with the help of powder X-ray diffraction analysis, thermogravimetric and Kurtz-Perry methods, respectively. The crystal was found to be in the mono crystal structure. The thermal studies of Thiourea tartrate reveals that at crystal is stable up to 208 ºC and shows absence of water molecules below 100 ºC. The NLO study measured with the help of Kurtz and Perry powder SHG technique and the results confirms that Thiourea tartrate has 1.6 times greater NLO efficiency than the KDP. Impedance analysis of the Thiourea Tartrate Sample has two semi circles which might be due to the contributions from grain and grain boundary. As grown Thiourea tartrate crystals can be used up to 2080C only for any applications and SHG results confirms the suitability of the crystals for NLO applications.

Keywords: Thiourea tartrate, XRD, Thermal Analysis, NLO.

INTRODUCTION

A nonlinear optical crystal importance arises in the wide areas that include second harmonic generation, frequency mixing, and electrooptic modulation. Recently, the thiourea complex crystals have attracted some special interest from the researchers on their nonlinear optical behavior (1). That such structural patterns arising out from an anion, like this monovalent tartrate anion may lead to infinite chains distinguished with very short O-H---O interactions between the dicarboxylate anions, may suggest certain promising ways in the introduction of new nonlinear optical material pathways. [2].

To achieve SHG, non-centrosymmetry is critical and this has been achieved in a variety of organic systems by a range of different approaches. Probably the most convenient method is through the use of a single enantiomer of a chiral component where the crystals are ensured to grow in an acentric space group (3). In this point of view, Thiourea tartrate single crystal was grown by the slow evaporation solution growth method. L (+) -tartaric acid is a strong organic acid. Some molecular salts based on derivatives of L(+) tartaric acid have been synthesized. Some of these exhibit higher

second harmonic generation efficiencies than urea. Among these latter compounds, 2-amino-5-nitropyridinium dihydrogen phosphate has an interesting nonlinear optical behavior. 2-amino-5-nitropyridinium L-nonhydrogen phosphate, urea-(+) tartaric acid and L-tartaric acid-nicotinamide, L-Histidine nitrate and L-Cystine tartrate monohydrate (4) and L-Polonium tartrate (5) are reported to be nonlinear optical materials. Also, researchers have reported the growth of L (+)-tartaric acid single crystal (6, 7).

Although the crystal structure and properties of numerous thiourea metal complexes have been reported (8-11). A study of single crystal growth of Thiourea with organic Tartaric acid is missing in the literature. In the present investigation attempts were made to grow good quality single crystals of Thiourea tartrate for Second harmonic generation applications and the grown crystals were characterized by XRD, FTIR, TGT-DTA and impedance analyzer, etc.,

EXPERIMENTAL

In the present work, we have grown thiourea tartrate single crystals using the slow evaporation method. The saturated solutions were prepared by mixing thiourea with tartaric acid in a 1:1 molar ratio in triple distilled water according to the given equation.

$$C_4H_6O_6 + CS\,[NH_2]_2 \rightarrow [CS\,[NH_2]\,C_4H_6O_6] \text{ - (1)}$$

Then the final solution was filtered using a filter paper and kept at room temperature. Furhter, repeated recrystallization were done to improve the purity of the crystals. As a result, optically transparent seed crystals without defects were obtained. Large single crystals of the salt are obtained by using a slow cooling process as shown in Fig. 1 in a constant-temperature bath made in the home lab.

This paper gauges the sufficiency of the crystal under study to pose as three-dimensional diffraction gratings for X-ray wavelengths. The exercise is carried out to study the structure and atomic spacing. The crystalline sample was exposed to constructive, concentrated monochromatic X-rays. The experimental setup was designed to comply the condition that the diffraction angle and the lattice spacing are related with the wavelength of electromagnetic radiation.

Figure 1: Thiourea Tartrate Crystal.

RESULT AND DISCUSSION

The crystal structure of the prepared materials was determined by the XRD studies. It confirms a small change in the lattice parameter values of the grown crystals. The X-ray powder diffraction of the powdered grown sample of Thiourea tartaric acid is shown in figure.2. The sharp peak confirms the good crystalline quality of the grown sample. The XRD pattern was compared with the reported JCPDS card nos. 5220179 and 791104. The calculated lattice parameters of the grown samples are tabulated in Table 1**.** The resultant values were used to plot a diffractogram as shown in the Fig.2.

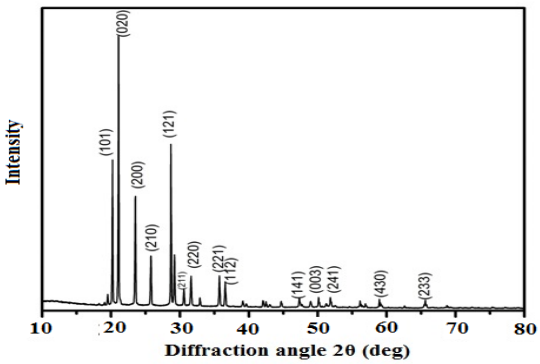

Figure 2: Powder XRD Pattern of Thiourea Tartrate.

Table 1: Crystallographic Characteristics

S.No.	Unit Cell dimensions
1	a = 6.01 Å
2	b = 6.91 Å
3	c = 8.11 Å
4	α = 90.00 °
5	β = 91.00 °
6	γ = 90.00 °
7	V = 337 $Å^3$
8	System = Monoclinic

In the present investigation, we decided to do Thermo gravimetric analysis (TGA) for Thiourea tartrate between room temperature between 27 °C and 800°C at a heating rate of 20 °C per minute and unfortunately at 208 °C sample exploded. Based on the previous records for both pure Tartaric acid and pure Thiourea spectrum was recorded up to 800 °C. But in the case of thiourea tartrate, the sample undergoes an explosive reaction as shown in Fig.3.

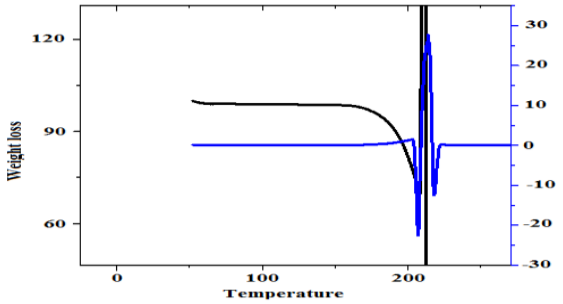

Figure 3: TG- DTA Spectrum of Thiourea Tartarate.

As the grown samples are needle shaped, it is very difficult to make parallel plate capacitor. Hence grown samples were made in to dense pellet and annealed at 60 ºC for 3 hr to remove moisture and density of pellet was increased. By coating silver paste on both sides of the pellet and it made as parallel plate capacitor. The measurements were made at different temperatures by Impedance Analyzer. An ideal Nyquist or Cole-Cole plot might show three semicircles with the contributions from the (1) bulk of the grain (2) grain boundary contribution and (3) Electrode contributions. The experimental spectra clearly show two different semicircles for the Thiourea Tartrate Sample which might be due to the contributions from grain and grain boundary. The measurement results are shown in Fig. 4.

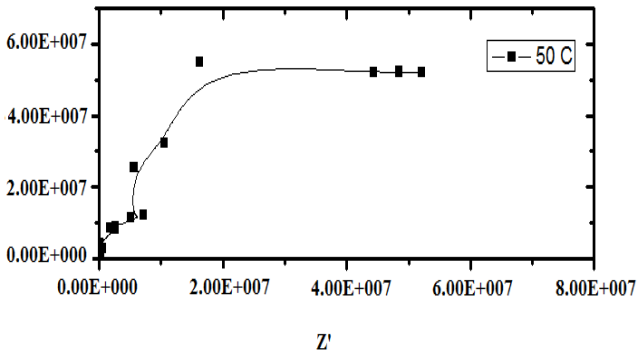

Figure 4: Cole-Cole Diagram of Thiourea Tartarate.

The powder second harmonic conversion efficiency of the Thiourea Tartrate sample was examined by Kurtz and Perry powder technique and the efficiency of the sample was compared with crystalline powder of KDP. A Q-switched, mode-latched Nd: YAG optical device operative at the elemental wavelength of 1.064 µm was used. Within the current investigation, the optical device pulse of 8 ns with a spot radius of 1 millimetre was used. The input ray of light was had the IR reflector then directed on the crystalline fine sample packed in a very tube The KDP and Urea were used as a reference material and the SHG relative efficiency of the Thiourea Tartrate was found to be 1.6 times greater than that of KDP (Table 2).

Table 2: SHG Studies of TTC

Sl. No.	Crystal name	Output power (milli joule)	Input power (joule)
1	Tartaric acid + Thiourea	14.5	0.68
2	KDP (Reference)	8.8	0.68
3	Urea (Reference)	8.9	0.68

CONCLUSIONS

Transparent, good quality, colourless single crystal of thiourea tartrate was grown by slow evaporation method. X-ray studies confirm compound formation without any impurity phase. TG-DTA analyses in the case of TTC crystals shows abrupt rise in values due to the explosion of TTC powders. Based on the TG-DTA results we are suggesting that thiourea tartrate single crystals cannot be used for any applications about 207°C. The SHG relative efficiency of the Thiourea Tartrate was found to be 1.6 times higher than that of KDP.

REFERENCES

[1] Sandhya Ravi and Chenthamarai S, Growth and Characterization of Single Crystals of Thiourea based compounds, Indian J. Sci. Res, 2014;9:051-057.

[2] Srinivasan TP, Anandhi S, and Gopalakrishnan R, Growth and characterization of 2-methylimidazolium d-tartrate single crystal, J. Cryst. Growth, 2011;318:768-773.

[3] Kotler Z, Hierle R, Josse D, Zyss J, and Masse R, Quadratic nonlinear-optical properties of a new transparent and highly efficient organic–inorganic crystal: 2-amino-5-nitropyridinium-dihydrogen phosphate (2A5NPDP), J. Opt. Soc. Am. B, 1992;9(4):534-547.

[4] Robert R, Justin Raj C, Krishnan S, Uthrakumar R, Dinakaran S, and Jerome Das S, Spectral, optical and mechanical studies on L-histidine hydrochloride monohydrate (LHC) single crystals grown by unidirectional growth technique, Physica B, 2010; 405:3248-3252.

[5] Natarajan S, Moovendaran K, Kalyana Sundar J, Bhagavannarayana G, and Martin Britto Dhas SA, Influence of picric acid on the SHG efficiency of L-prolinium tartrate crystals, J. Miner. Mater. Charact. Eng., 2011;10: 913-921**.**

[6] Begum S.A, Hossain M, and Podder J, An investigation on the growth and characterization of thiourea single crystal grown from aqueous solutions, J. Bangladesh Acad. Sci., 2009; 33:63-70.

[7] Renuka Kadirvelraj, Arun M. Umarji, Ward T. Robinson, Santanu Bhattacharya, and Tayur N. Guru Row, Systematic Crystallographic Investigation of Hydrogen-Bonded Networks Involving Monohydrogen Tartrate−Amine Complexes: Potential Materials for Nonlinear Optics, Chem. Mater. 1996;8:2313-2323.

[8] Krishna Mohan M, Jagannathan K, Ponnusamy S, and Muthamizhchelvan C, Effect of urea and thiourea on nonlinear optical hippuric acid crystals, J. Phys. Chem. Solids, 2011;72:1273-1278.

[9] Renuka Kadirvelraj, Arun M. Umarji, Ward T. Robinson, Santanu Bhattacharya, and Tayur N. Guru Row, Systematic Crystallographic Investigation of Hydrogen-Bonded Networks Involving Monohydrogen Tartrate−Amine Complexes: Potential Materials for Nonlinear Optics, Chem. Mater., 1996;8: 2313-2323.

[10] Heng-Yun Ye, Da-Wei Fu,Yi Zhang,Wen Zhang , Ren-Gen Xiong, and Songping D. Huang "Hydrogen-Bonded Ferroelectrics Based on Metal−Organic Coordination" J. Am. Chem. Soc. 2009;131(1):42–43.

[11] Greg Brewer, Raymond J. Butcher and Peter Zavalij, Use of Pyrazole Hydrogen Bonding in Tripodal Complexes to Form Self Assembled Homochiral Dimers, Materials (Basel). 2020;13(7):1595.