GROWTH AND CHARACTERIZATION OF PURE THIOUREA DOPED WITH SODIUM CHLORIDE CRYSTAL

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ABSTRACT

Poly crystals of pure thiourea doped with sodium chloride an organic material: have been grown by slow evaporation technique at room temperature . The functional group of the grown crystals was found by FTIR analysis. The spectral bands have been compared with similar thiourea complexes using FTIR spectrum in the range 400- 3600 cm^{-1} .The UV- Vis study was performed to know optical behaviour of the grown crystals.

I.INTRODUCTION

The search for new organic nonlinear optical crystals has been of great interest because of their wide range of potential applications such as frequency doubling, optical switching, optical disk data storage, optical modulation, laser remote sensing and medical diagnostics. These materials attracting significant attention as they posses large nonlinear optical susceptibilities, ultrafast nonlinear response time, high laser damage threshold and scope for introducing desirable characteristics by multifunctional substitutions [1-3]. For NLO device applications still there is a demand for good quality crystals with higher efficiency. For the past ten years amino acids are playing a vital role in the nonlinear optical crystal growth. They individually exhibit nonlinear properties as they posses proton donor carboxyl acid (COO^-) and proton acceptor amino (NH_3) group also in solid state they exist as zwitterions. Amino acid crystals play a major role in NLO applications such as L-valine, L-alanine, L-proline, L-leucine, L-histidine, L-arginine and L-phenylalanine. Worldwide urea and its derivatives are extensively used in crystal engineering and supramolecular chemistry for their flexibility in the synthesis of functional materials. Also for a long time it is used as a model system for crystals from solution growth and reference material in Powder SHG .In the present work urea and L-valine single crystals were grown by slow evaporation solution growth technique. The grown crystal was characterized by various characterization techniques such as CHN analysis; powder XRD, FT-IR,UV- Vis analysis.

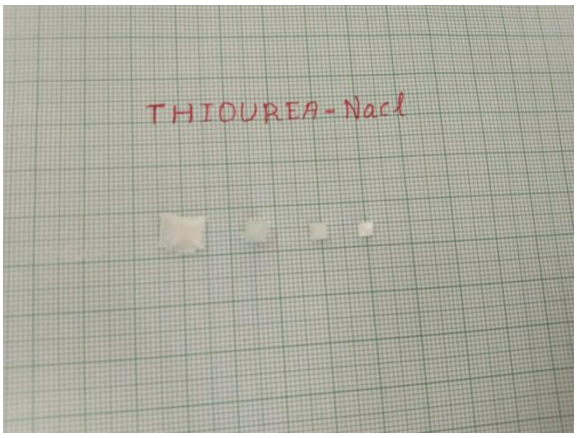
II . METHODS

(1) Slow Evaporation Method:

In this method, an excess of a given solute is established by utilizing the difference between the rates of evaporation of the system remains constant in the solvent evaporation method. The solution loses particles, which are weakly bound to other components and therefore the volume of the solution decreases. In almost all cases, the vapour pressure of the solute and therefore the solvent evaporates more rapidly and the solution becomes supersaturated usually it is sufficient to allow the vapour format above the solution to escapes freely into the atmosphere. This is the oldest method of crystal grown by 15 days and technologically. It is very simple typical growth conditions involve temperature stabilization to about 0.005^0C and rates of evaporation of a few mm^3/hr.

GROWTH OF PURE THIOUREA CRYSTAL:

The present work is aimed to the growth of **Thiourea Doped Sodium chloride Crystals** In this work, Thiourea [$C_5H_6N_2O_2$] is doped with Sodium chloride [Na Cl] was used to grow crystal from solution growth technique. The saturated and the supersaturated solution were prepared



Grown crystals of Thiourea doped sodium chloride crystal.

The FTIR spectra of as prepared pure Thiourea crystal sample:

The FTIR spectrum of the T-NaCl crystal is shown in figure 5.1. The FTIR spectrum exhibits strong and medium modes of hydroxyl groups. The high intensity in the FTIR spectra of the bands at 3391cm^{-1} and 1270cm^{-1} indicates the crystalline of the crystal in the xrd pattern. The observed frequencies of the T-NaCl crystal are given in the following table.

Frequency(cm^{-1})	**Nature of the peak**	**Assignment**
3391.89	STRONG	O-H STRETCHING
2192.82	STRONG	C-H STRETCHING
1616.34	STRONG	RING STRITCHES
1467.93	VARIABLE	C=O ASYMMETRIC SKETCHES
1412.99	STRONG	CH_2 BENDING
1270.01	MEDIUM	CH_2 BENDING
1050.85	MEDIUM	SHOULDER WITH ASYMMETRIC SKETCHES
824.81	WEEK	CO- STRETCHING

The graph is plotted between % transmittance and wave number (cm-1).In this graph different peaks formed at different intensity (a.u). It is observed in the graph that pureThiourea doped with sodium chloride have various frequency vibrations which are shown by different peaks.

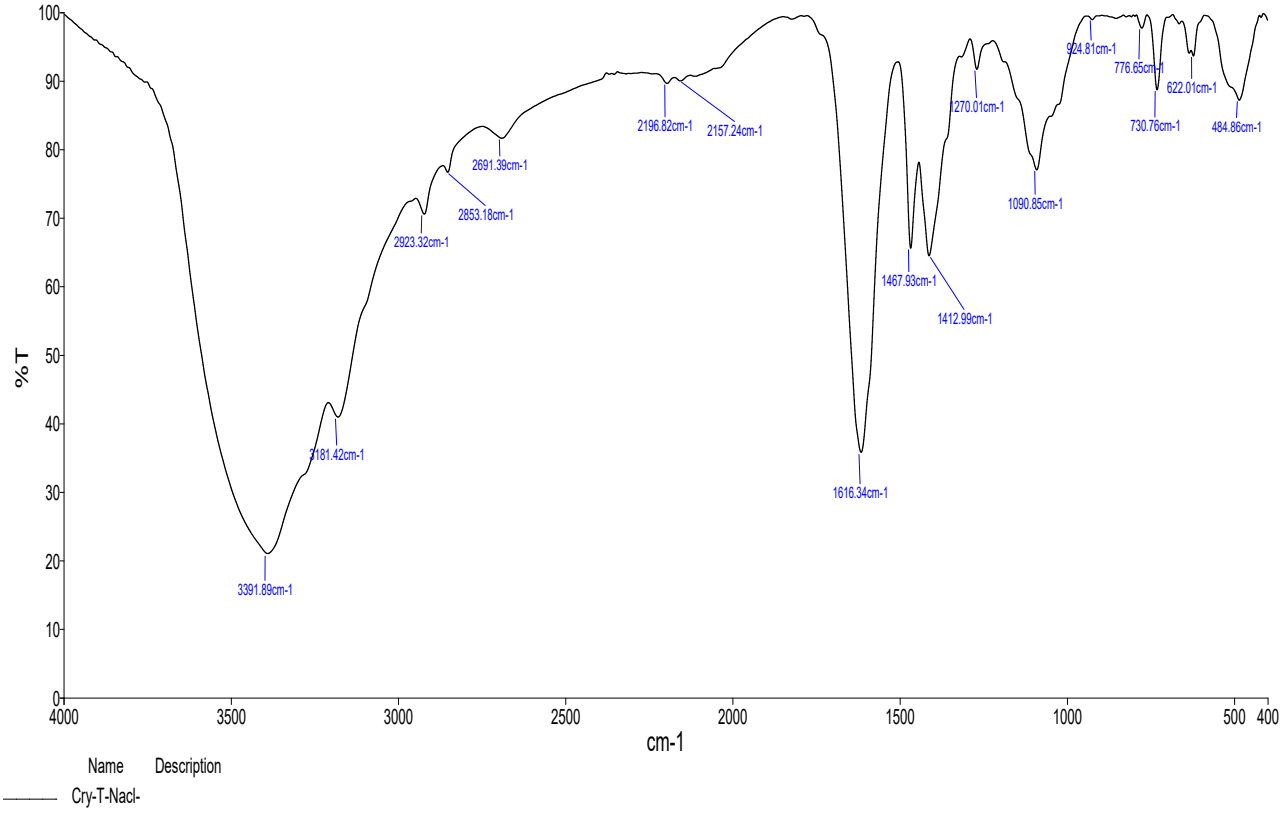
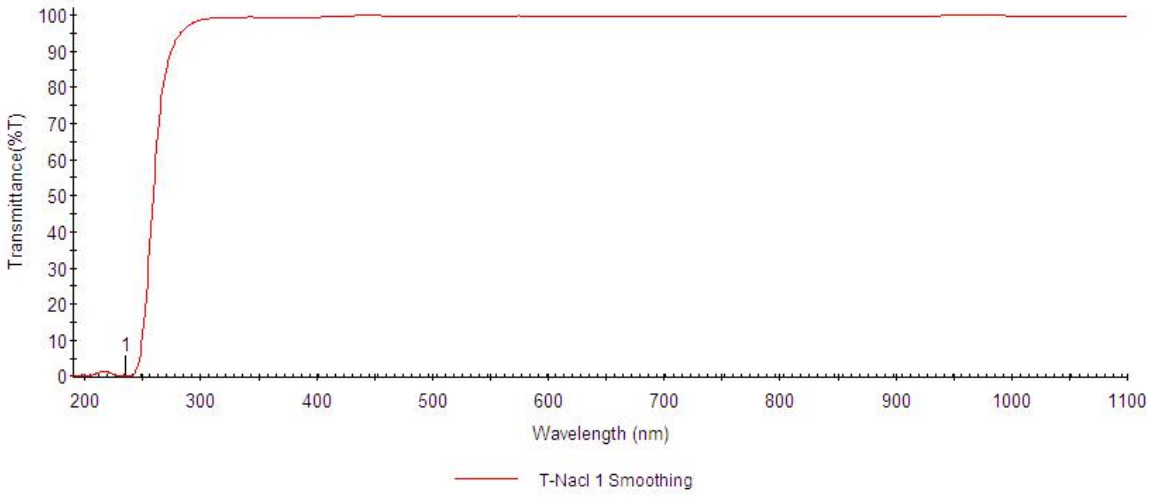


Figure: FTIR spectrum of the T-NaCl crystals

The UV spectra of as pure Thiourea doped sodium chloride crystal sample:

The optical transmission studies were recorded for the sample obtained from the crystal. The sample is prepared by dissolving in the water. To find the transmission range of pure Thiourea doped with sodium chloride crystal the optical transmission spectrum was recorded using UV –Vis Nir spectrometer. The UV cut-off wavelength for the crystal is 270nm and the crystal is found to be transparent from the region 300nm to 1100nm is key element for the requirement of NLO properties.



Name	No. Peak(nm)	Peak(%T)
T-Nacl	235.35	0.0131

CONCLUSION

The NLO crystals of thiourea doped with sodium chloride T-NaCl (were synthesized by using slow evaporation method in the ratio of 1:1. The properties of the thiourea and sodium chloride crystal were studied by using Fourier Transform Infrared spectroscopy (FTIR), and UV-Visible spectroscopy analysis.

The FTIR spectrum exhibits strong and medium modes of hydroxyl groups. The high intensity in the FTIR spectrum at 3391cm^{-1} and 1616cm^{-1} indicates the crystalline of the crystal.

The UV transmittance spectrum reveals the optical properties of the T-NaCl crystal. The UV cut off wavelength is at 260nm and transmittance ranging from 200nm-1100nm. The NLO properties of the crystal are confirmed by its transparency in the UV spectrum.

Thus T-NaCl crystal can be used for NLO applications and by further studies it can be proved for many other applications in the field of biomedical, laser and optical.

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