# UV, FTIR, TGA-DSC and NLO Studies of Ammonium Chloride Doped L-Threonine Crystals

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**Abstract**

Ammonium chloride doped L-Threonine crystals have been grown by slow evaporation solution growth technique successfully. The optical properties such as transparency and SHG efficiency were diagnosed by UV-Vis-NIR and NLO spectral studies. The structural property and thermal stabilities of the grown crystal by solution growth were analyzed by X-ray TGA-DSC studies. Presence of the functional groups was estimated using FTIR spectral analysis which gave a confirmation about the presence of ammonium in the newly grown crystal.

**Keywords:** UV-Vis-NIR, FTIR, XRD, TGA-DSC and NLO.

## 1. Introduction

Generally, compounds based on amino acid are capable of NLO behavior by producing SHG which exposed the usefulness in the fabrication of photonic, optoelectronic and switching devices. Researchers focused their efforts on metal mixed organic amino acid crystals for the enhancement of mechanical strength, chemical stability, and SHG or THG properties. Amino acid crystals doped with metal ions or in pure form were grown by several researchers and lot of studies were carried out (1-4). Necessity arises to fabricate a new NLO material for Opto-electronic, Photonic devices etc., L-Threonine along with various dopants has been reported as a very good NLO material with a promising SHG efficiency which was highly pronounced on compared with KDP,ADP and Urea etc,(5-9). Ammonium Chloride doped L-Threonine can be synthesized for the growth of a new NLO material with an expectation of a pronounced SHG efficiency. Adopting solution growth slow evaporation technique ammonium chloride doped L-Threonine crystal has been successfully grown is reported in the current study.

UV-Vis-NIR spectrum, FTIR, TGA-DSC and NLO characterization studies reveals the newly grown crystal is a special one with predictable enhanced physical and chemical properties leads to an idea for device fabrication to satisfy the modern era scientists. Due to the non-volatile crystalline nature, high thermal stability, insoluble in non-polar solvents and are easily soluble in water determines that the amino acid crystals are the most suitable material for a new NLO crystals to satisfy all optical applications (10-14).

## 2. Experimental

2.1 Synthesis

Single crystal of L-Threonine doped with ammonium chloride were grown by slow evaporation solution growth process from the aqueous solution obtained by dissolving AR grade L-Threonine available commercially in double distilled water along with ammonium chloride(). The saturated solution was stirred for about 30 minutes using magnetic stirrer and was kept in a beaker closed with a perforated pin holed plastic paper for about 40 days. Doped crystals of L-Threonine are which are seems to be highly transparent and with predictable quality crystals. The hardness and stability are also found to be increased due to the inclusion of dopant.

## 3. Results and Discussions

### 3.1 UV-Vis-NIR spectral analysis

The UV-Vis-NIR spectrometer of LAMBDA 35 is used to evaluate the absorption and transparency of the grown material of L-Threonine doped with ammonium chloride by recording the optical transmittance and absorption spectra within a range of 200 – 1100nm. 226nm is the lower cut off wavelength for the grown ammonium chloride doped L-Threonine crystal with a range of transparency between 220-1100nm as shown in the figure 1 & 2. The wide transparency range made a foundation that the grown crystal should possess a very good dielectric nature which will results in induced polarization mechanisms leads to NLO activity on the exposure of intense radiation on the crystal. The second harmonic generation efficiency of a crystal depends on the better conversion ability.

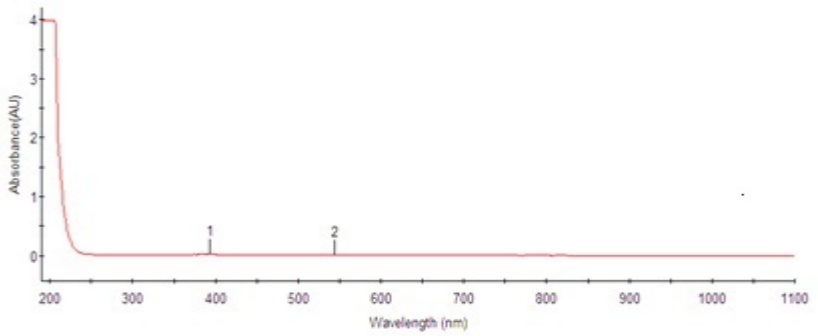


Figure 1. UV-Vis absorbance spectrum of Ammonium Chloride Doped L-Threonine Crystal

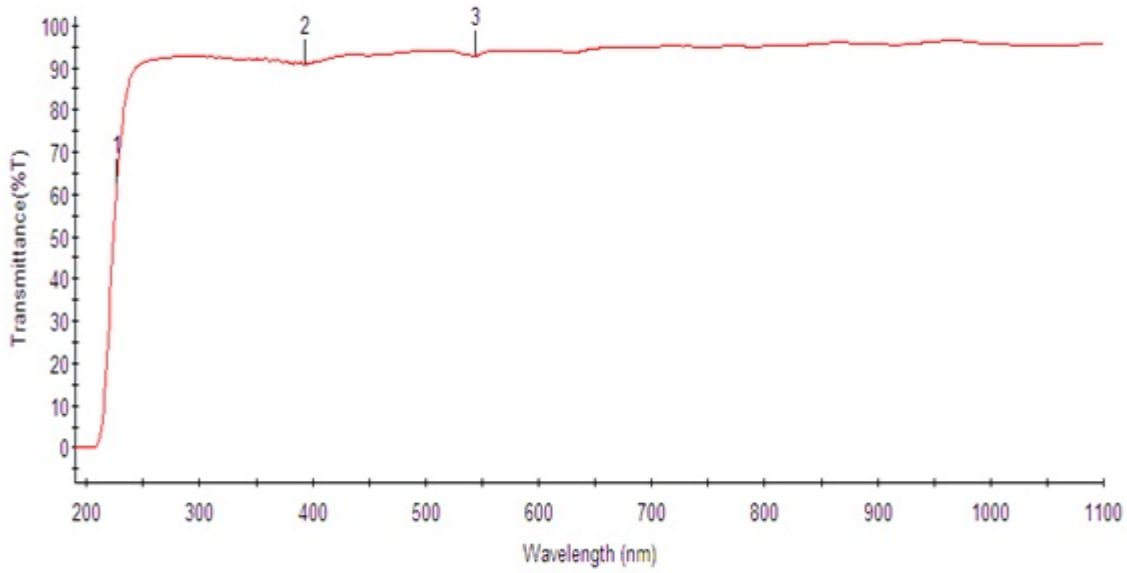


Figure 2. UV-Vis transmittance spectrum of Ammonium Chloride Doped L-Threonine Crystal

### 3.2 FT-IR spectral analysis

Infra-red spectroscopy confirms the presence of functional groups. FTIR spectrum alone can provide more information about the compound on compared with other available electronic spectra. The absence or presence of absoption bands will help to predict the functional groups presence in the compound. From the reported values it was confirmed that L-Threonine structure consists $NH_3$(amine),two CH groups, carboxylic groups, C=O, two CH groups and $CH_3$.Ammonium Chloride presence was confirmed with the impact due to the internal vibrations of NH4 group and N-Cl stretching which results in pronouncement of thermal stability. The upstream shift of $\gamma_1$-doubly degenerate N-H oscillation occurs at 3029$cm^{-1}$ and an additional peak found at 710$cm^{-1}$ gave the information about the additional N-Cl assigned stretching. Finally it is presumed that the grown crystal of ammonium chloride doped L-Threonine would be a coordinated compound along with its dopant (ammonium ion). The variations and occurrence of shift confirms clearly about the inclusion.

| Wavenumber($cm^{-1}$) | Tentative Asignments |
|---|---|
| 3029 | $\gamma_1$-doubly degenerate N-H oscillation |
| 2874 | CH Stretching |
| 2977 | CH asymmetric stretching |
| 1629 | $NH_2$ deformation(asymmetric) |
| 1457 | $NH_2$ deformtion (Symmetric) |
| 1417 | $CH_3$ asymmetric bending |
| 1345 | $CH_3$ symmetric bending |
| 1184 | Rocking of $NH_3$ |
| 1113 | Rocking of $NH_3$ |
| 1040 | Stretching of CN |
| 932 | C-C Stretching |
| 701 | N-Cl Stretching |
| 560 | C-C-N deformation |
| 489 | Torsion mode of $NH_3$ |

Table.1 FTIR data table of Ammonium Chloride doped L-threonine.

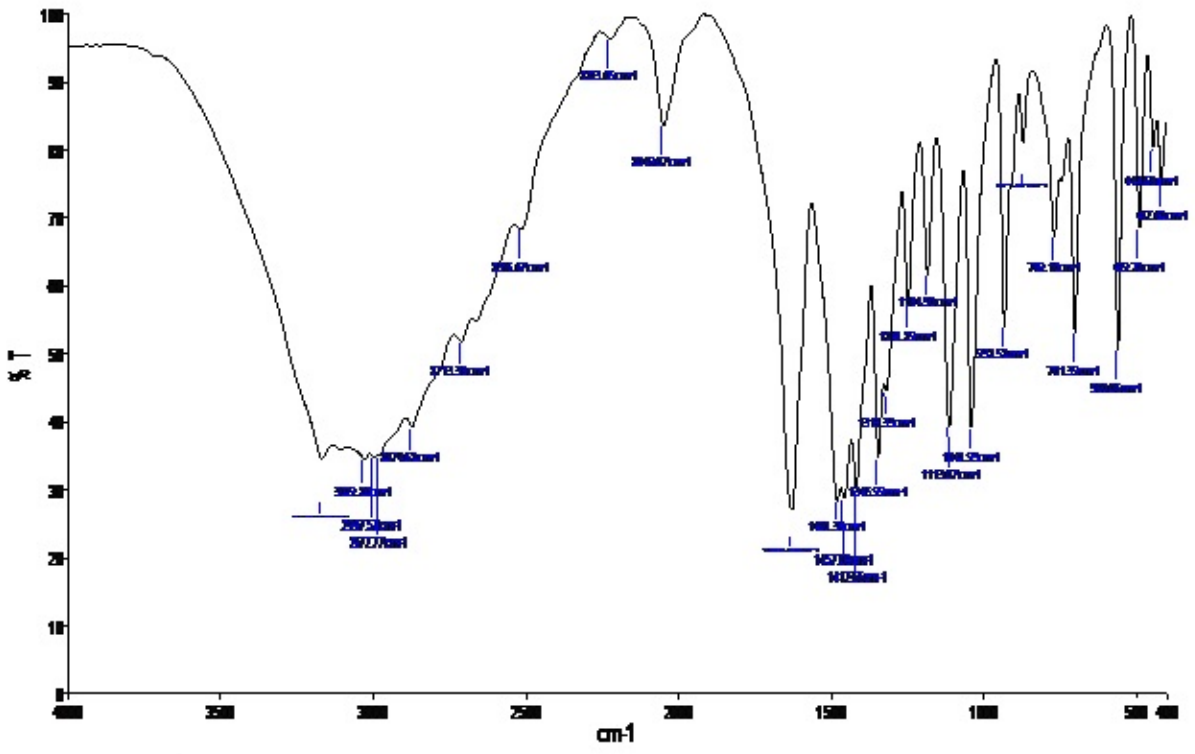


Figure 3. FT-IR spectrum of Ammonium Chloride Doped L-Threonine Crystal

### 3.3 Thermal Analysis

The DSC-TGA curves of ammonium chloride doped L-Threonine crystal recorded in nitrogen gas environment with a heating rate 10°C/min are shown in the figure .4 within a temperature range of 0°C to 300°C. From the TGA curve it was observed that occurrence of weight loss starts at 215 °C and ends at 237° C. A single stage decomposition takes place at 215°C and weight loss occurs on continuous heating confirming the maximum decomposition of the grown crystal takes place only around 237°C.. This DSC-TGA analysis confirms that the grown ammonium chloride doped L-Threonine crystal is stable up to 215°C and may be utilized for NLO high power laser applications up to its thermal stability.

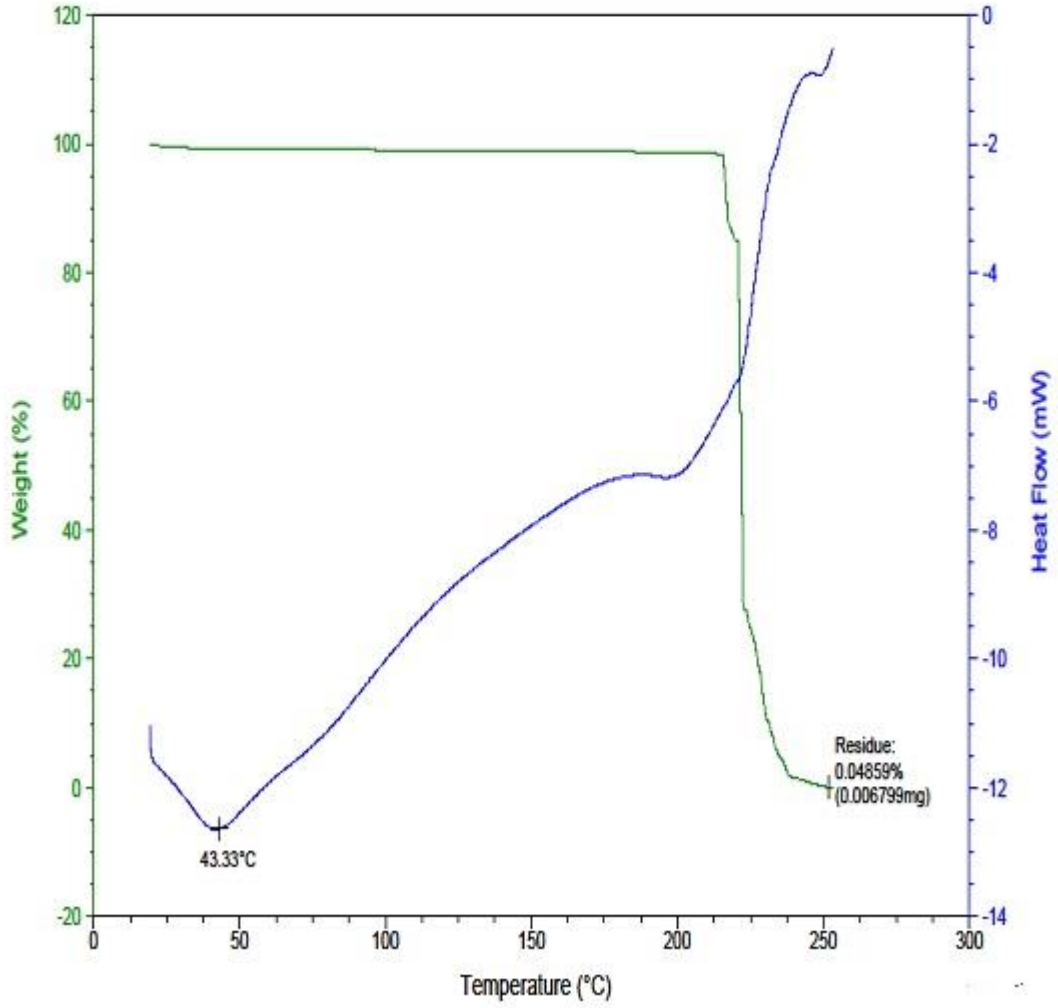


Figure 4. Thermal studies of Ammonium Chloride Doped L-Threonine Crystal

### 3.4 Second Harmonic Generation

To confirm the NLO (nonlinear optical) property of the grown ammonium chloride doped L-Threonine crystal, Technique of Kurtz and Perry powder was used. A Q-switched laser source of 1064nm emitted wavelength from Nd:YAG laser source was used to illuminate the sample with a pulse width of 8 nanoseconds. Emission of green light from the powdered crystal sample kept in the holder which was made to expose on the path of laser confirms the efficiency of second harmonic generation .The output was measured as 10mJ with an incident input energy of 0.681mJ/pulse on the sample. The output of the grown crystal is found to be 1.12 times greater than the standard KDP material. The SHG efficiency of the ammonium chloride doped L-Threonine crystal will confirms that the crystal must be a promising material of NLO due to its nonlinear and linear optical properties.

## 4. Conclusion

Single crystals of ammonium chloride doped L-Threonine have been grown at room temperature by slow evaporation solution growth technique. The lower cutoff wavelength (226nm) and the high transparency of the grown crystal prove that the new trail with ammonium chloride dopant gave an outcome as prominent potential material for the fabrication of NLO device. The DSC-TGA analysis confirms the thermal stability up to 215°C and the crystal may be used under a operating temperature in device fabrication for the applications up to 215°C. A very good SHG output made a foundation about the device fabrications which will be utilized in the field of opto-electronic communications.

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