Research Article www.ijcps.com

International Journal of
Chemical and Pharmaceutical Sciences
2015, Dec., Vol. 6 (4)

ISSN: 0976-9390

IJCPS

Synthesis Growth and Characterization of a new NLO material: L-Threonine Lithium Chloride

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Received: 19th Nov 2015, Revised and Accepted: 22nd Nov 2015

ABSTRACT

A new NLO material L-Threonine Lithium Chloride was grown from aqueous solution by a slow evaporation technique at room temperature. Crystals were characterized by X-ray diffraction analysis whose results they crystallize on orthorhombic system. The UV-Visible spectroscopic study reveals that crystal has good optical transparency and lower cut-off wavelength was found to be 330nm. The functional group of grown crystal was found by FTIR analysis. The nonlinear optical property was confirmed by Kurtz Perry powder technique..

Keywords: L-Threonine Lithium Chloride, XRD, UV-Visible Spectroscopy, FTIR, NLO.

1. INTRODUCTION

Materials with second order of non-linear optics have greatly attracted due to their possible applications in new technologies of optoelectronics [1-3]. Organic materials have been of particular interest, since non-linear optical responses on these materials are of microscopic origin, thus offering an opportunity to utilize theoretical models along with synthesis flexibility to design and produce new materials [4,5]. Most of the organic crystals have inadequate transparency, poor optical quality and low laser damage threshold [6]. Moreover, growth of large sized single crystals has excellent mechanical and thermal properties but they possess relatively modest nonlinearity. Due to the above reasons, a lot of research has been carried out on semi organic materials which have combined properties of both organic and inorganic materials [7]. Amino acids have interest applications on Non-Linear Optics (NLO) because they are materials of second order [8]. One of their properties is that they are non-volatile crystalline solids, melting at relatively high temperatures; they are insoluble in non-polar solvents and they are soluble in water, so their aqueous solutions behave like solutions with elevated bi-polar momentum. L-Threonine crystallizes with four zwitterionic molecules per unit cell linked by a three dimensional network of NH…O and O-H…) bonds. L-Threonine is one of the essential amino acid bearing an alcohol group. Also, optically active amino acids contain many highly efficient optical second-harmonic generators and are promising candidates for a great number of applications. By the physical point of view the L- Threonine Lithium Chloride investigation is relevant both owing to the possibility to observe the behaviour of a system where the hydrogen bond plays a fundamental role [9,10] and the technological importance of a material which shows second-harmonic conversion efficiency greater than 1 relative to potassium dihydrogen phosphate.

2. EXPERIMENTAL

2.1. Crystal growth

Single crystals of L-Threonine Lithium Chloride was grown by preparing L-Threonine and Lithium Chloride taken in 1:1 equimolar ratio in deionised water at room temperature and stirred well to yield a homogeneous mixture of solution. The solution was filtered to remove insoluble impurities using Whatman filter paper of pore size 10 micrometers. Then the solution of

L-Threonine Lithium Chloride was taken in a beaker with a perforated lid in order to control the evaporation rate and kept at room temperature for crystallization. Finally a well defined single crystal was obtained after 15 days by slow evaporation method. The photograph of the grown crystal of L-Threonine Lithium Chloride is shown in figure1.

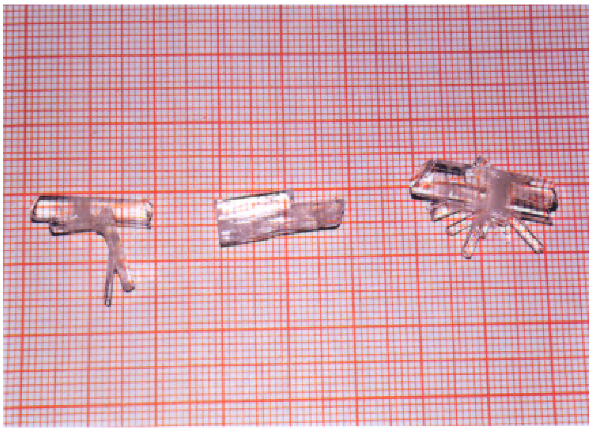

Figure - 1: Morphology of L-Threonine Lithium Chloride Single Crystal.

2.2 Characterization Methods

Powder X-ray diffraction study of the grown crystal was carried out using Bruker's X-ray diffractometer. The optical absorption spectra of the grown crystals were recorded using Perkin Elmer Lambda 35 model UV-Visible spectrometer in the wavelength region 190-1100nm. The FTIR spectrum of L-Threonine Lithium Chloride was recorded by PERKIN ELMER RX9 spectrometer using KBr pellet technique in the wavelength range 4000-400cm^{-1}.

3. RESULTS AND DISCUSSION

3.1 Powder X-ray diffraction studies

Powder X-ray diffraction study of the grown crystal was carried out by using Bruker's X-ray diffractometer (Figure 2). XRD analysis has confirmed that the crystal belongs to orthorhombic with space group $P2_12_12_1$. The space group suggests that the grown material is non-centrosymmetric which fulfils the fundamental criterion for the material to exhibit NLO behaviour.

3.2 UV-Visible spectral analysis

The UV-Visible transmission spectrum is very important for optical material because of its wide transmittance window. The high transparency was confirmed from the recorded spectrum and it was observed that there was no significant absorption in the range 320-1100nm (Figure 3). There is an advantage in the use of amino acids, where the absence of strongly conjugated bands leads to a wide transparency range in the visible and UV spectral regions. The lower cut-off was found to be around 320nm which combined to good transparency attests to the usefulness of L-Threonine Lithium Chloride material for optoelectronic application.

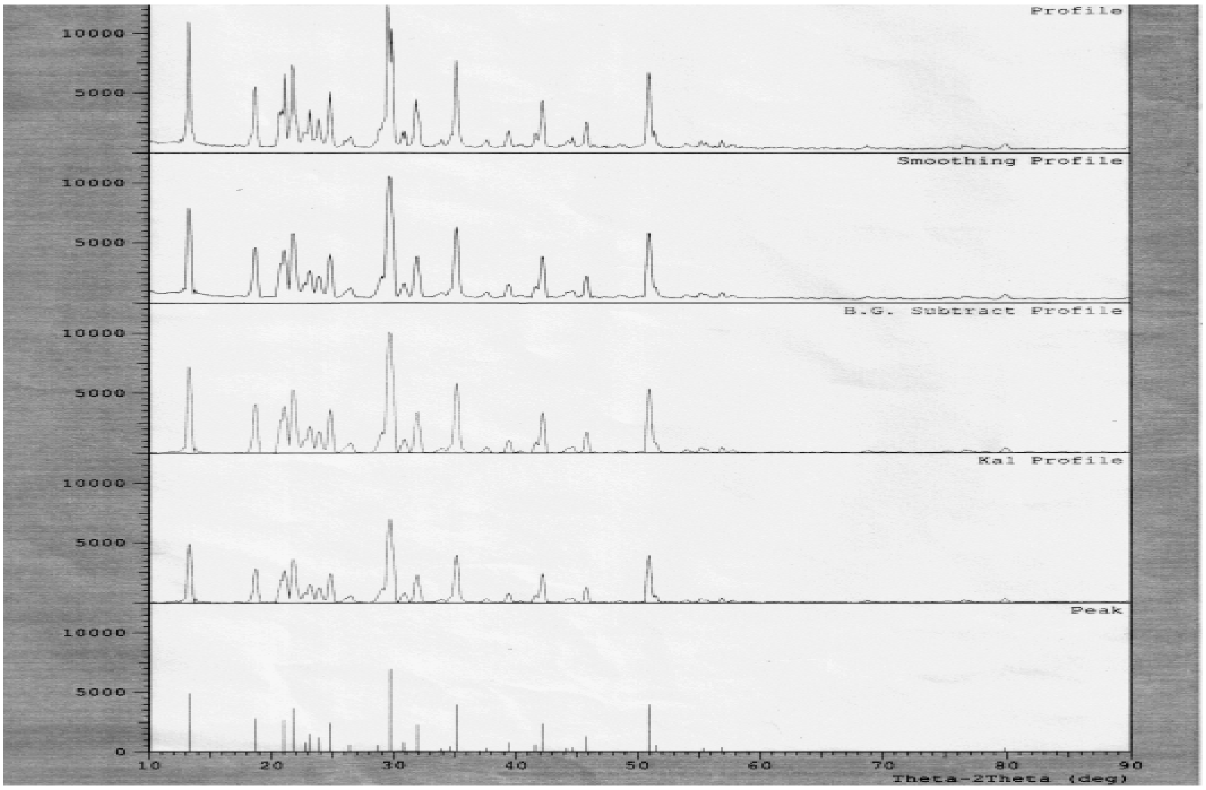

Figure - 2: X-ray diffraction pattern of L-Threonine lithium chloride.

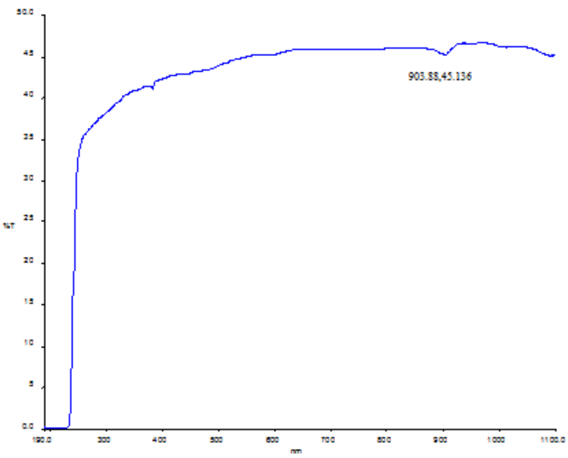

Figure – 3: UV –Visible spectrum of L-Threonine lithium chloride.

3.3. FTIR Spectroscopic analysis

The FTIR spectrum of the sample was recorded in the frequency region of 4000-400 cm^{-1} using PERKIN ELMER RX9 FTIR Spectrometer to confirm the vibrational structure of grown crystalline compound. Figure 4 shows the FTIR Spectrum of L-Threonine Lithium Chloride. The broad absorption of medium intensity peaks at 3169.91 and 3030.16cm^{-1} was assigned due to NH_3^+ asymmetric and symmetric stretching vibration. Due to the stretching vibration involving carbon and nitrogen of amino group exist a peak at 1039.90cm^{-1}. The asymmetric NH_3^+ deformation occurs at 1629.23cm^{-1}. The absorption peak at 1480.44 cm^{-1} was due to symmetric NH_3^+ deformation vibration. The peak at 1416.97cm^{-1}reveals the COO^- symmetric vibration. The peak at 2874.52 cm^{-1}indicates the C-H stretching vibration. The NH_3^+ rocking vibration was observed at 1247.73 and 1113.05cm^{-1}. The C-C-N deformation was observed at 559.27cm^{-1}. Hence, the presence of functional groups was confirmed from the above assignments.

Table - 1: Vibrational assignments of L-Threonine Lithium Chloride single crystal

Wave number cm^{-1}	Vibrational assignments
3169.91	NH_3^+ asymmetric stretching
3030.16	NH_3^+ symmetric stretching
2874.52	C-H symmetric stretching
1629.23	NH_3^+ asymmetric deformation
1480.44	NH_3^+ symmetric deformation
1416.97	COO^- asymmetric stretching
1247.73, 1113.05	NH_3^+ rocking
559.2	C-C-N deformation

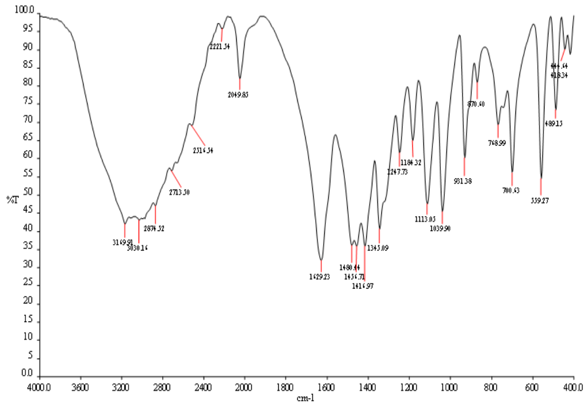

Figure – 4: FTIR spectrum of L-Threonine lithium chloride single crystal.

3.4 NLO Test

The SHG behaviour of the powdered material was tested using Kurtz Perry method [11]. The sample was ground into very fine powder and tightly packed in a micro capillary tube. Then it was mounted in the path of Nd:YAG laser beam of 9.6 mj pulse energy obtained by splitting the original laser beam. The output light was passed through monochromator which was detected green light at 532 nm. This confirms the NLO behaviour of the material. The green light intensity registered by a photomultiplier tube and converted into an electrical signal. The same particle size of KDP was used as a reference material. SHG efficiency of L-Threonine Lithium Chloride was greater than that of KDP.

4. CONCLUSION

Single crystals of L-Threonine Lithium Chloride were grown by slow evaporation technique. Powder XRD confirms the orthorhombic structure of the crystal. FTIR analysis confirms the presence of functional groups present in the crystal. The optical transmittance of the crystal was found to be around 330nm. SHG efficiency shows that the crystal has a higher efficiency than KDP.

5. REFERENCES

1. Madhurambal G, Mariappan M, Hariharan S, Ramasamy P and Mojumdar SC. **J Therm Anal and Calorim,** 2013; 112(2): 1127.
2. Ravindran B, Mariappan M, Ramamurthi K and Mojumdar SC. **J Therm Anal and Calorim,** 2011; 104 (3): 875.
3. Sangeetha MK, Mariappan M and Madhurambal G, Mojumdar SC. **J Therm Anal and Calorim.** 2012; 108(3): 887.

4. Mojumdar SC, Madhurambal G, Mariappan M and Ravindran B. **J Therm Anal and Calorim,** 2011; 104(3): 901.
5. Jiang MH and Fong Q. **Adv. Mater.** 1999; 11: 1147.
6. Ravindran B, Madhurambal G and Mariappan M, Ramamurthi K, Mojumdar SC. **J Therm Anal and Calorim,** 2011; 104(3): 909.
7. Franken PA, Hill AE, Peters CW and Weinreich G. **Phys. Rev. Lett.** 1961; 7: 118.
8. Madhurambal G, Mariappan M, Hariharan S, Ramasamy P and Mojumdar SC, **J Therm Anal and Calorim,** 2013; 112 (2): 1031.
9. Madhurambal G, Ravindran B, Mariappan M and Mojumdar SC. **J Therm Anal and Calorim,** 2011; 108 (3): 905.
10. Sangeetha MK, Mariappan M, Madhurambal G and Mojumdar SC. **J Therm Anal and Calorim,** 2013; 112 (2): 1059.
11. Kurtz SK and Perry TT. **J Appl Phys.** 1968; 39 (8): 3798.