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Growth of Lithium Sulphate doped L-threonine for the study of Bioactivity and NLO behavior

J. Elberin Mary Therasa[1]*, D. Jayaramanb[1], V. Josepha[2]
[1]Department of Physics, Loyola College, Chennai, Tamil Nadu, India
[2]Department of Physics, Presidency College, Chennai, Tamil Nadu, India
***Corresponding author: E-Mail: elberinraj@gmail.com**

ABSTRACT

Lithium Sulphate doped L-threonine (Li_2SO_4-LT), a semi-organic material, has been synthesised and grown by slow evaporation technique at room temperature. The grown crystals were subjected to single crystal X-ray diffraction analysis in order to establish their crystalline nature. Li_2SO_4-LT crystal belongs to the orthorhombic crystal system with space group $P2_12_12_1$. The antimicrobial screening tests were recorded by Agar well diffusion method to analyze the biological activity. The second harmonic generation (SHG) efficiency was measured by the Kurtz and Perry powder technique using Nd: YAG laser and was found to be 1.46 times that of standard potassium dihydrogen phosphate (KDP).

KEY WORDS: Slow evaporation, X-ray diffraction, Bioactivity, NLO property.

1. INTRODUCTION

The importance of amino acid for NLO applications is due to the molecular chirality, absence of strongly conjugated bonds and zwitterionic nature of the molecule. L-threonine molecule can exist in zwitterionic form and hence it is capable of forming compounds with anionic, cationic and neutral chemical compounds. Owing to its basic nature, L-threonine forms a number of salts with different organic and inorganic acids and many of them are found to show evidence of interesting NLO properties. The grown crystal was subjected to XRD study to determine the lattice parameters to confirm the title compound. Besides NLO applications, the grown material shows moderate antibacterial and antifungal activities. Hence, this material has the combined advantages of nonlinear and bioactive properties. Therefore, in the present work, single crystals of Li2SO4-LT were grown. Bioactivity and Nonlinear optical studies were carried out to analyze the antibacterial and antifungal activities and SHG efficiency of the grown material.

2. EXPERIMENTAL

2.1. Synthesis and growth of Li_2SO_4-LT: The compound Li_2SO_4-LT was synthesized by the reaction of L-threonine with lithium sulphate. A saturated solution of lithium sulphate was prepared and L-threonine was added slowly at room temperature. The solution was stirred for 12 hours to get homogeneity. The homogeneous solution was filtered and kept undisturbed for slow evaporation at room temperature. After a period of one month, the crystals were harvested. The grown crystals were purified by recrystallization process. The photograph of the as-grown doped crystal with the dimensions of 30×5×3 mm^3 is shown in Fig.1.

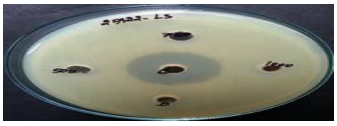
Fig.1.Photograph of as - grown Li_2SO_4-LT single crystal

3. RESULTS

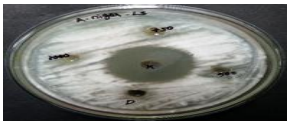
3.1. Single crystal X-ray diffraction study: The grown crystal was subjected to single crystal X-ray diffraction studies using Bruker X8 Kappa APEXII single crystal X-ray diffraction. From the diffraction analysis, it has been found that the title compound crystallizes in orthorhombic system, with non-centro symmetric space group, $P2_12_12_1$. The lattice parameters were estimated as a=7.66Å, b=5.27Å, c=13.61Å, with the unit cell volume of 549$Å^3$. The deviation in cell parameters from those of L-threonine confirms the dopant in the host material.

3.2. Bioactivity study:

Antibacterial and Antifungal activities: The sample screening for antibacterial and antifungal activity against human pathogens such as *E.coli* (ATCC 25922) and *Aspergillus niger* was made using Agar well diffusion method. Three different concentrations of samples (500, 750 and 1000µg/100µl/well) were used in the present investigation. Muller Hinton Agar (MHA) plates were incubated with test organisms. The plates were evenly spread out. Then wells were prepared in the plates with a cork borer. Each well was loaded with 0.1ml of corresponding concentration of sample and Chloramphenicol was used as a positive control for antibacterial activity and Ketoconazole was used as a positive control for antifungal activity. The plates were incubated for 24hrs at 37°C. The development of inhibition zone around the well was measured and recorded.



2(a).Antibacterial activity of the sample Li_2SO_4-LT



2(b).Antifungal activity of the sample Li_2SO_4-LT

Figs. 2(a) and (b) show three different concentration of antibacterial and antifungal activity of the sample Li_2SO_4-LT (500, 750, 1000 µg/100µl/well) by Agar well diffusion method. The results of the antibacterial and antifungal screening by Agar well diffusion method are shown in Table.1. The antibiotic screening for the complex is clearly noted through the dimension of the inhibition zone. The inhibition zone is found to increase with increase, in the case of antibacterial activity for the bacterial species *E.coli* (ATCC 25922). It is also observed that the complex shows moderate antibacterial activity in comparison with standard antibacterial agent Chloramphenicol.

Table.1.The antibacterial and antifungal activities of Li_2SO_4-LT crystal

Organisms	Concentration	Zone of inhibition (mm)	
		Li_2SO_4-LT	Standard(positive control)
E.coli	500	No result	30
	750	10	
	1000	11	
Aspergillus niger	500	8	35
	750	10	
	1000	11	

In the case of antifungal activity also, the inhibition zone is found to increase with increase of concentrations for the antifungal species *Aspergillus niger*. Hence, the complex shows moderate antifungal activity in comparison with standard antifungal agent Ketoconazole. It is concluded that the grown material can show moderate antibacterial and antifungal activities.

3.3. NLO property: The nonlinear optical property was tested using Kurtz and Perry powder technique. The crystal was ground into a homogeneous powder and densely packed between two transparent glass slides of a cell. A Q-switched Nd: YAG laser (DCRII) was used as light source. A laser beam of fundamental wave length 1064 nm, 8ns pulse width with 10 Hz pulse rate was allowed to strike the sample cell normally. The power of the incident beam was measured using a power meter. The green light was detected by a photomultiplier tube. The SHG output (10.07 mV) was finally detected using a photomultiplier tube. KDP crystal was powdered to the identical size and was used as reference material to detect the SHG output (6.9 mV). The SHG efficiency of doped Li_2SO_4-LT crystal was found to be 1.46 times higher than that of KDP. Therefore it is concluded that the doped crystal is a potential nonlinear optical material with more efficiency.

4. CONCLUSION

Single crystals of Li_2SO_4-LT were grown by slow evaporation technique within a period of 1 month. The doped crystal was subjected to single crystal X-ray diffraction and it was confirmed that the crystal belongs to the orthorhombic system with space group $P2_12_12_1$.The results of the antibacterial and antifungal activities show that the grown crystal possesses moderate biological activity against the bacterial and fungal species. The second harmonic generation (SHG) efficiency was measured by the Kurtz and Perry powder technique using Nd:YAG laser and was found to be 1.46 times that of standard potassium dihydrogen phosphate (KDP). Hence, the grown material can be considered as one of the potential NLO candidates for the fabrication of electro-optic nonlinear optical applications involving frequency-doubling process. Further, it can show antibacterial and antifungal activities in pharmaceutical applications.

5. ACKNOWLEDGEMENT

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