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Study on Growth, Structural and Optical Properties of L-Alanine Doped Nickel Sulphate Hexahydrate Single Crystals

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Abstract: ***L-Alanine doped NSH single crystals were grown by slow evaporation technique for different molar concentrations (0.01, 0.03, 0.05).The grown crystals were subjected to various studies. The crystal structure is determined by single crystal X-ray diffraction at room temperature. The LANSH crystal belongs to the tetragonal space group. The functional groups of the grown crystals were predicted by FTIR analysis. Optical transparency of grown crystals has been analysed by UV-Vis-NIR spectral studies.***

Keywords: Crystal growth, X-ray diffraction, FTIR, UV-VIS-NIR studies

1. Introduction

Crystal growth and characterization is one of the important research area in science and technology. Developments in technology have stimulated the importance of discovering new materials and modifying the already known materials. Growth of single crystals and their structural and physical characterization come under the scientific research on crystalline materials. Single crystals are important materials for electronic, optical devices and laser crystals. In recent years several studies dealing with organic inorganic and semi organic molecules and materials called nonlinear optics (NLO) are being reported due to the increasing need for photonic applications. The nonlinear responses induced in various molecules in solution and solids are of great interest in many fields of research [1-3]. Crystalline semi-organic salts of amino acids have recently attracted considerable interest among researchers. The amino acid group materials have been mixed with inorganic salts to form adducts or complexes in order to improve their mechanical, thermal and NLO properties [4-8]. In the present investigation the single crystal of pure Nickel Sulphate Hexahydrate and L-Alanine doped Nickel Sulphate Hexahydrate was grown by slow evaporation method. Nickel sulphate Hexahydrate (NSH) crystals are widely used for UV light filters and UV sensors [9-11].

2. Crystal Growth

The title compound was prepared by dissolving analar grade Nickel Sulphate Hexahydrate (NSH) by means of doping it with L-Alanine in different but definite molecular ratios. We have grown pure and L-Alanine doped crystals by the slow evaporation method at room temperature. NSH crystal was doped with L-Alanine in three NSH:L–Alanine molecular ratios, viz. 1:0.01, 1:0.03 and 1:0.05.Approximate molar ratio of materials was taken using digital balance and dissolved in double distilled water. The solution was stirred with magnetic stirrer and allowed to evaporate without disturbance. Optically good quality NSH single crystals have been grown within a period of 55-61 days. Initially very small crystals appeared then grew bigger in size. Out off grown crystals, best crystals were selected for further studies and are shown in Figure 1.

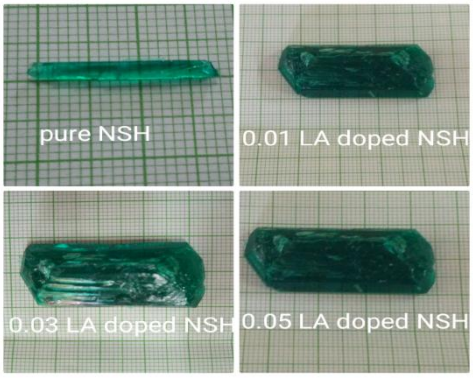

Figure 1: Grown crystals of Pure and doped NSH Crystals

3. Characterizations

The PXRD data were collected from powdered sample for pure and doped NSH crystals using diffractrometer. The reflections were indexed. Analysis of the X-ray peaks was done by available methods and lattice parameters were determined [1, 3, 3]. Infrared spectroscopy is an extremely effective method for determining the presence or absence of a wide variety no of functional group in a molecule. In the present study, FTIR spectrum was recorded in order to qualitively analysed the presence of functional groups.UV visible study of the grown crystal was carried out by Lambda-35 UV visible spectrometer in a range 200-500nm. Optically clear L-Alanine doped NSH single crystals was used for this study.

4. Results and Discussion

4.1 Powder XRD

X-ray diffraction studies of solution grown NSH crystals was carried on XPERT-PRO using X-ray CuKα radiation (1.54059340) was used. The samples were scanned in the 2Θ range of 10^0-70^0 X-ray diffract to gram is shown in figure2. The technique is based on observing the scattered intensity when X-ray beam is incident on a sample. It is a function of incident and scattered angle, polarization, and wavelength or energy[12]. The figure2 shows the powder X-ray diffraction pattern, the presence of prominent Bragg's peak 2Θ angle confirms the perfect crystal line structure. Table1 indicates the unit cell parameters satisfy the condition for Tetragonal system i.e., a=b≠c and $\alpha=\beta=\gamma=90^0$ from the above data and it may be concluded that the grown crystals of NSH have tetragonal system with very slight changes in the peak positions, slight change in the relative intensities, cell volume. and lattice parameters and these slight changes are due to the doping of L-Alanine in NSH crystals.

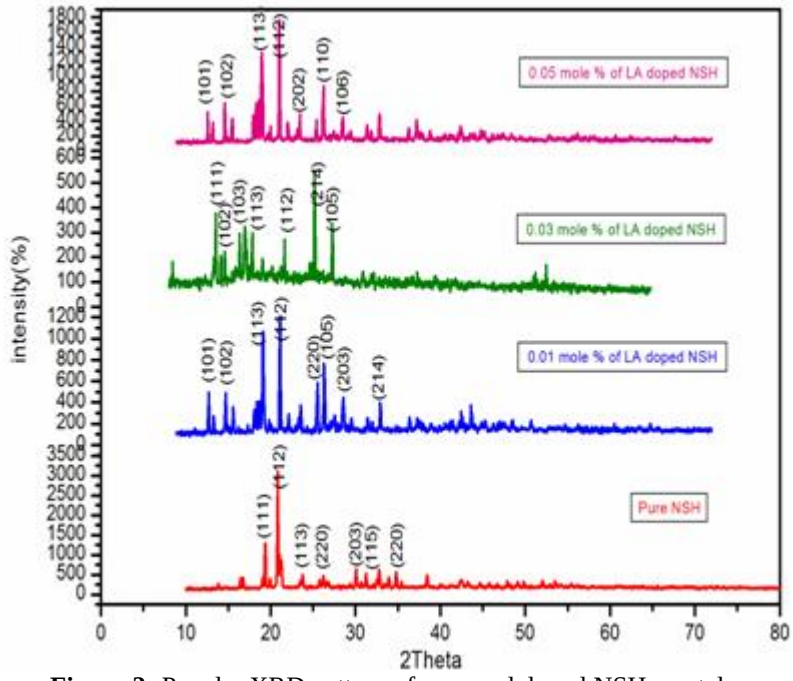

Figure 2: Powder XRD pattern of pure and doped NSH crystals

Table 1: Calculated Lattice parameter for pure and doped NSH single crystals

Samples	Crystal system	Unit cell parameter			Volume
		A=B	C		
Pure NSH	Tetragonal	6.773	18.176	$\alpha=\beta=\gamma=90^0$	834.98
AD1(0.01 mole% of L-Alanine doped NSH)		6.665	18.544		834.65
AD2(0.03 mole% of L-Alanine doped NSH)		6.644	18.355		834.47
AD3(0.05 mole% of L-Alanine doped NSH)		6.658	18.448		834.55

4.2 Fourier Transform Infrared Spectroscopic Studies

Infrared spectroscopy is an extremely effective method for determining the presence or absence of a wide variety no of functional group in a molecule. In the present study, FTIR spectrum was recorded in order to qualitively analysed the presence of functional groups in L- Alanine doped NSH single crystals in the range 400cm^{-1} to4000 cm^{-1} using Perkin Elmer grating infrared spectrophotometer.

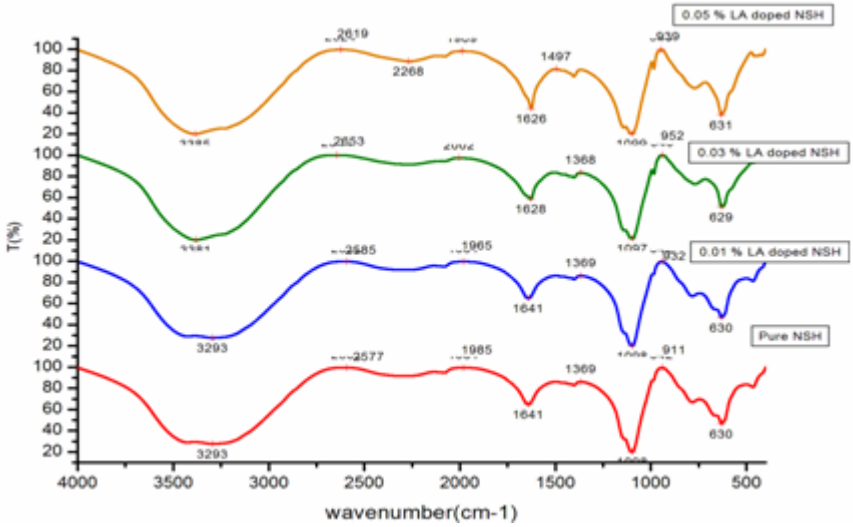

Figure 3: FTIR spectrum of L-Alanine doped NSH single crystal

Table 2: The functional groups assignments L-Alanine doped NSH single crystals

FTIR Wave numbers (cm^{-1}) for				Assignments
Pure NSH	L-Alanine doped NSH			
	AD1	AD2	AD3	
3362	3293	3381	3385	O-H Stretching
2601	2592	2644	2624	CH_3 Stretching
2258	-	-	2268	C=N Stretching
1953	1981	2002	1989	C-H bending
1625	1641	1628	1626	C=C Stretching
1368	1369	1368	-	C-H Rocking
1101	1098	1097	1099	C-N Stretching
951	942	940	946	NH_3 bending
631	630	629	631	C-Cl Stretching vibration

4.3 UV- Visible Spectral Analysis

The UV-VisNIR spectroscopy of the pure and doped NSH crystals was performed by using Double Beam Spectrophotometer. The crystals have a good optical absorbance in the entire visible region and the lower cut off wavelength is observed. The band gap energies were calculated and presented in Table3 and Figure4 showed the UV absorbance and True plots. The single crystals are mainly used for optical applications. The UV Vis NIR absorption spectra are observed in the present study. The lower cut off region lies in the range 394 nm. The grown crystals has good absorbance in UV as well as in visible regions.

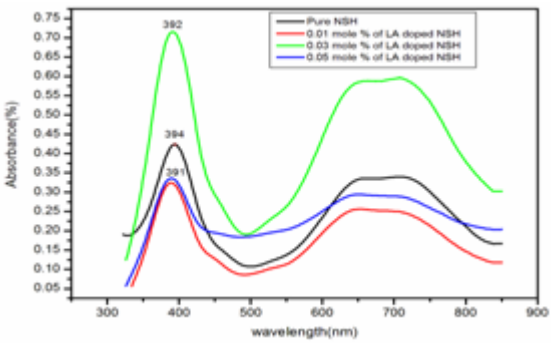

Figure 4: UV-Vis-NIR spectroscopy of the pure and doped NSH crystals

Table 3: Results of Band gap Energy

System	*λcut (nm)*	*Eg (eV)*
Pure NSH	394	3.153
AD1(0.01 mole % of LA doped NSH)	391	3.177
AD2(0.03 mole % of LA doped NSH)	392	3.169
AD3(0.05 mole % of LA doped NSH)	391	3.177

5. Conclusion

Single crystals of L-Alanine doped NSH were grown by Slow Evaporation method at room temperature. Powder X-ray diffraction studies were carried out for L-Alanine doped NSH single crystals and the lattice parameters were calculated. PXRD analysis revealed that the grown crystals belong to Tetragonal system. The FTIR spectrum reveals that the various functional groups present in the grown crystal .The FTIR studies assign vibrational frequency. From the UV spectrum, the L-Alanine doped NSH single crystal is found to be absorbance in the UV region and it could be a useful candidate for opto electronic application in visible and infrared region.L-Alanine doped NSH single crystal is transparent and found an application in optical studies. The optical band gap is found to be 394nm.The optical absorbance spectrum of L-Alanine doped NSH single crystal 3.15eV.

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