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GROWTH AND CHARACTERIZATION OF SEMI-ORGANIC NLO MATERIAL: SERINE SODIUM CHLORIDE (SSC)

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ABSTRACT

Single crystals of Serine Sodium Chloride (SSC), a semi organic nonlinear optical material has been grown from solution by slow evaporation at ambient temperature. The growth of crystals has been carried out at various pH values and the growth was confirmed at pH 5.7. The chemical composition of the grown crystals was determined by the FTIR spectra. The crystalline nature was confirmed by single crystal XRD. The crystal system was found to be orthorombic. The structure is built from alternate layers of Serine organic molecules and inorganic layers consisting of Na^+ ions and Cl^- ions. The SHG was confirmed using the Kurtz powder technique.

Keywords: Semi Organic; Nonlinear Optical; Slow Evaporation; Inorganic Layers; Grain Size; SHG

INTRODUCTION

In recent years, organo-inorganic hybrid materials have attracted considerable attention. In particular, the inorganic derivatives of protein amino acids are often attributed to symmetric groups without an inversion centre mostly to polar symmetry groups. Their crystals have properties whose symmetry is described by odd -rank tensors such as pyro-electric effect, spontaneous electric polarization, piezoelectric effect, generation of second optical harmonics, etc. Moreover crystals that belong to the eleven enantiomorphic point groups, having no mirror reflection planes exhibit optical activity, which is described in terms of the axial generation tensors. While the structures of most amino acids are well defined, the structures of the derivatives of the protein amino acids with inorganic components are not. This paper defines the crystal structure of Serine Sodium Chloride [SSC]. This has been investigated by the FTIR studies, its crystalline nature is studied by the single crystal XRD, the transmittance and absorbance of electromagnetic radiation is studied through UV-Visible spectrum.

EXPERIMENTAL

Synthesis and crystal growth

SSC was synthesized from analytic grade of Serine and Sodium Chloride (Merck) in equimolar ratio and dissolved in triple distilled water. The pH of the solution at super-saturation is kept at 5.7. The solution is filtered and transferred to a Petri dish for crystallization. This compound is re-crystallized 2 times for purity. Then the pure samples of seed crystals are taken and characterized.

Characterization

The crystals were characterized by FTIR spectroscopy, single crystal XRD and UV-Visible spectroscopy. FTIR spectra were recorded on Shimadzu IFS 66V FTIR.

Single crystal XRD was obtained on a PHILIPS X'PERT MPD system.(Table 1) The absorption spectrum for the title crystal was recorded using JASCO corp., V-570, and Rev.1.00 UV-VIS spectrometer in the region 190-2500nm . The crystals were evaluated by the Krutz and Perry (1968) powder technique using a Q-switched, mode locked Nd: YAG laser. A micro-crystalline material of KDP available at the Indian Institute of Science was used for comparison in the SHG measurements.

FT-IR Analysis (Figure 1)

The grown crystals were subjected to FT-IR analysis with sample prepared with KBr in the palletized form. The FT-IR spectrum of Serine Sodium Chloride was recorded in the region 4000-400cm^{-1}

employing Shimadzu IFS 66V spectrometer. The presence of OH is indicated by the broad absorption range 3463 cm^{-1} to 2264 cm^{-1}. C = C is absent. The absorption at a 1650 cm^{-1} is absent. The region between 3463 cm^{-1} to 2264 cm^{-1} also shows the absorption due to CH. The absorption at 3383 cm^{-1}, 1638 cm^{-1} and 1469 cm^{-1} conforms NH stretching C= O stretching ,may also be conformed by the absorption at 1345 cm^{-1} and 1223 cm^{-1} .The CH_2 stretching vibrations may be conformed by the following bands 917 cm^{-1} , 680 cm^{-1}, 610 cm^{-1} , 574 cm^{-1} , 525 cm^{-1}reported in the literature[1,2] (Table 2)

UV-Visible Spectrum Analysis (Figure 3)

The optical absorption spectra of Serine Sodium Chloride crystals (SSC) were recorded in the range 190 – 2500nm using Varian Carry 5E spectrophotometer. The fig shows the UV-Visible spectrum recorded with highly transparent single crystal of SSC of thickness 2mm. It is seen from the absorption spectrum the crystal is highly transparent after 300nm without any absorption peak, which is an essential parameter of NLO crystals. The absence of absorption of light in the visible region is the intrinsic property of the amino acids.

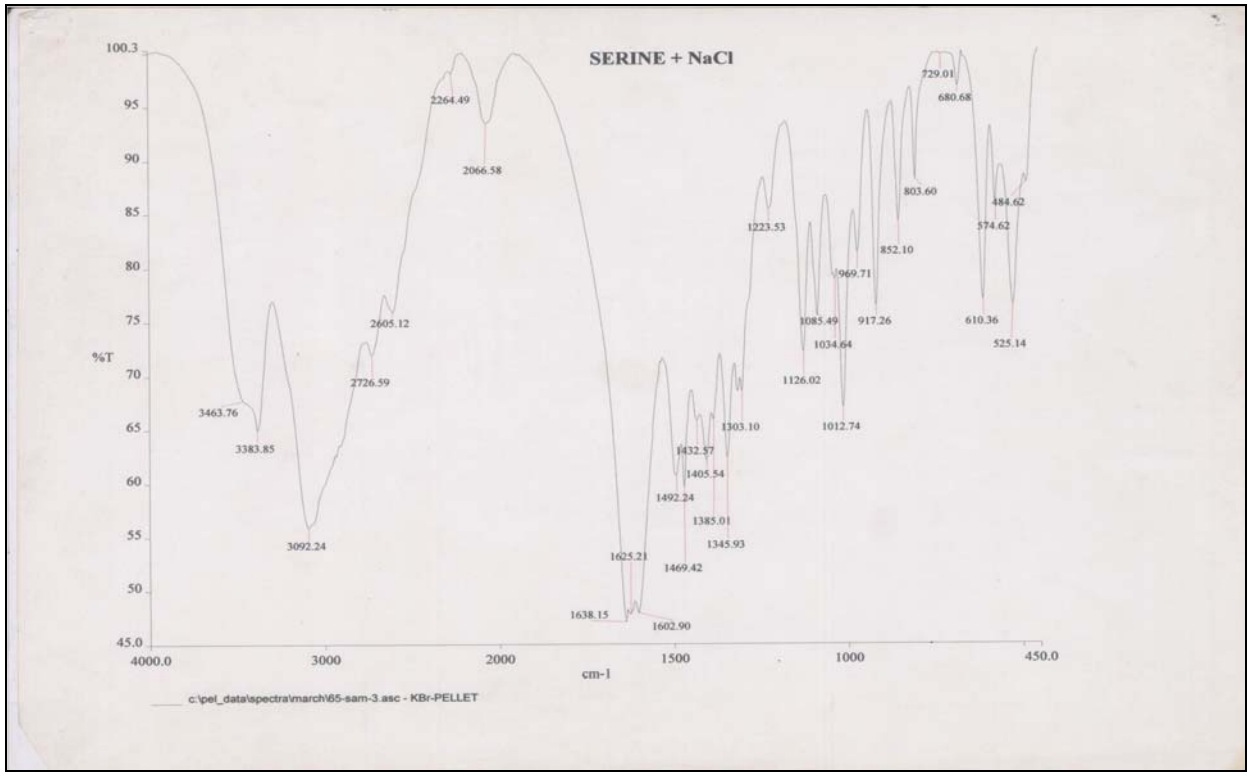

Fig.-1: FTIR Spectrum of Serine Sodium Chloride

NLO Studies

The NLO property of the crystal was confirmed by Kurtz powder technique. The determination of SHG intensity of the crystals using powder technique was developed by Kurtz and Perry[5] .The crystals are ground to powder and packed between two transparent glass slides. The first harmonic output of 1064 nm from a Nd:YAG laser was made to fall normally on the prepared sample with a pulse width of 8 ns. The second harmonic signal generated in the crystal was confirmed from the emission of green radiation by the sample. It is found that the SHG efficiency of the crystal is one and a half times higher than that in the case of KDP, which is in agreement with literature[1,4]. (Table 3)

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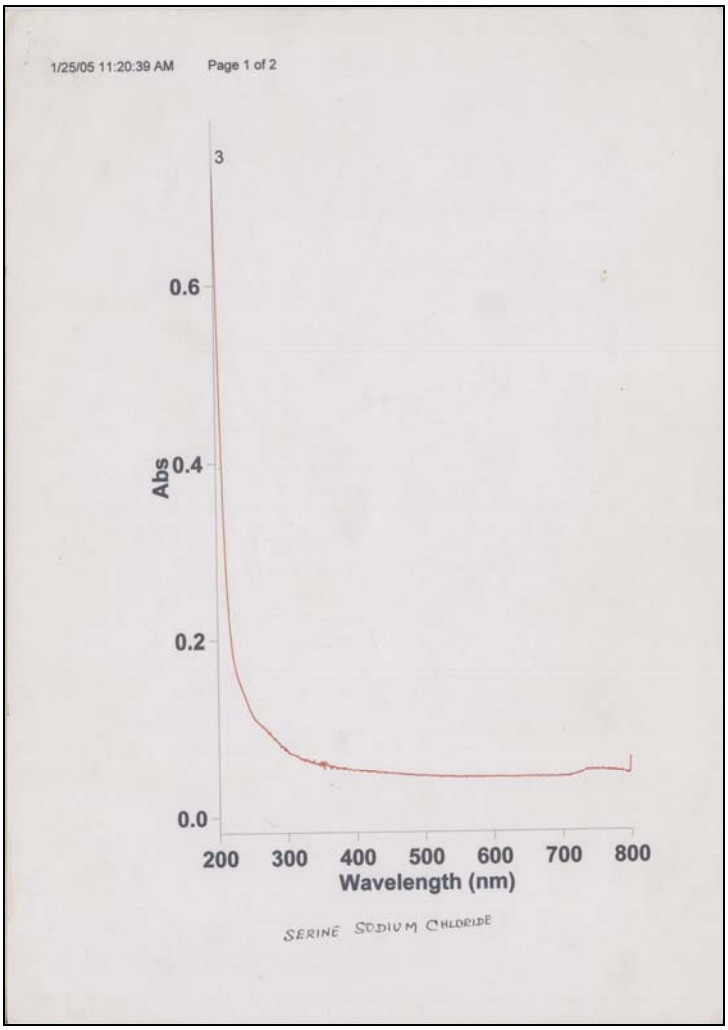

Fig.-2: UV-VIS spectrum of Serine Sodium Chloride crystal

Table-1: Single Crystal XRD data of Serine Sodium Chloride

a	**b**	**c**	**α**	**β**	**γ**	**Volume (A^O)**
5.6116 Aº	8.5685 Aº	9.3480 A^0	90^0	90^0	90^0	449.4775

The crystal System is Orthorombic.

Table-2: Frequencies of the fundamental vibrations of SSC

Frequency in wave number (cm^{-1})	**Assignment of vibration**
3464(s)	N-H stretching
3384(s)	NH_3^+ asymmetry stretching
3092(s)	NH_3^+ stretching
2726(m)	C-H stretching (Fermi resonance stretching
	of C-H and first overtone of C-H plane bending)
2265 (m)	Medial alkyne (disubstituted)
2067(w)	Isothiocynate(-NCS)
1638(s)	Open chain imino (-C=N-)
1625(s)	Secondary amine, NH stretch
1603(s)	Open chain azo (-N=N-)
1492(s)	Aromatic nitro compounds
1346(s)	-C-N stretch aromatic primary amine
1303(s)	-C-N stretch aromatic primary amine
1224(w)	Aromatic ethers, aryle –O stretch
1126(m)	Tertiary amine, C-N stretch
1085(m)	C-O stretch
1034(m)	Primary amine C-N stretch
1013(s)	Primary amine C-N stretch
970(m)	Trans C-H out of plane bend

Table-3: Power output of SHG signal developed in the KDP and the SSC crystals

KDP	**SSC pH = 5.7**
mW	**mW**
150	200
290	310
330	290

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