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FTIR Spectroscopic Studies on the Complex of Dl-Methionine with Trichloreacetic ACID

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ABSTRACT

The main objective of this present work is to grow a single crystal of complex DL-METHIONINE with TRICHLOREACETIC ACID and to investigate with FTIR spectroscopy.

Keywords: Solution growth, FTIR, Vibrational Spectra.

I. INTRODUCTION

Crystal:

A crystal is a solid in which the constituent atoms, molecules or ions are packed in a regular order with repeating pattern extending in all three spatial dimensions. The word crystal originates from the Greek word " Krystallos" meaning " clear ice", as it was thought to be especially solid form of water. Most metals encountered in everyday life are poly crystals. Crystals are often symmetrically inter grown to form crystal twins [3]. Crystal refers to solid objects that exhibit well-defined and often pleasing geometric shapes. Many types of crystals are found in nature. Snow flakes, diamonds and common salts are common examples of crystals.

Crystallography

To acquire fundamental data and to explore the properties of any solid state device, good quality single crystal is essential. Hence crystal growth has become the most vital and fundamental part of material science, engineering, physical science, biology etc. Single crystals of SiC, Ga As, InP are in great demand. Crystallography is the scientific study of crystals and crystal formation. It is often employed by materials scientists. The understanding of crystal structures is an important prerequisite for understanding crystallographic defects. A number of physical properties are linked to crystallography.

Crystal Structure

The process of forming a crystalline structure is often referred to as crystallization. While the cooling process generally results in generation of crystalline material, under certain conditions, the fluid may be frozen in a non-crystalline state. Crystalline structure occurs in all classes of materials, with all types of chemical bonds. Almost all metal exists in a polycrystalline state; amorphous or single crystal metals must be produced synthetically, often with great difficulty. In a single crystal, the crystal lattice of the entire sample is continuous and unbroken to the edges of the sample, without any grain boundaries. But a polycrystalline sample is made up of number of small crystals known as crystallites.

Crystal Growth Techniques

The main categories of crystal growth techniques are:

1. Solid growth: It involves solid – solid phase transitions.
2. Melt growth: It involves liquid – solid phase transitions.
3. Vapour growth: It involves vapour – solid phase transitions.

4. Solution growth: Growth of solute from an impure melt.
5. Gel growth: Alternative technique to solution growth.

II. METHODS AND MATERIAL

Low Temperature Solution Growth – Slow Evaporation Method

This is the oldest method of crystal growth and technically very simple. In this method, an excess of a given solute is established by utilizing the difference between the rates of evaporation of the solvent and the solute. In this method, the solution loses particles, solvent evaporates more rapidly and the solution becomes super saturated. Growth conditions involve temperature stabilization to about $+0.005^{\circ}$ C – 0.005° C and rate of evaporation is of few mm^3 / hr.

DL – Methionine is a sulfur-containing amino acid that is soluble in water. It involves more biological activity. Trichloro acetic acid is a strong organic acid used in organic synthesis and is an excellent medicine for wrinkles formed in the skin.

Transparent, colourless single crystals of DL-Methioninium trichloro acetate $(C^5H^{12}NO^2S)^+$ $(C^2Cl^3O^2)^-$ were crystallized at room temperature by slow evaporation from an aqueous solution containing DL- Methionine and trichloroacetic acid in a stoichiometric ratio of 1:1.

III. RESULTS AND DISCUSSION

Studies of vibrational spectra of amino acids by Infrared spectroscopy gives information regarding the behavior of normal modes, molecular confirmation, and effect of inter molecular forces and nature of hydrogen bonding on these biological fundamental substances. FTIR studies were carried out by Tandon et al., on poly L – Methionine [6]. S. Pandiarajan et.al., [5] presented the Infrared spectroscopic study of L – Methioninium nitrate. In the present investigation, the infrared spectroscopic analysis of DL- Methioninium trichloro acetate crystal was undertaken in the support of its crystal structure [7].

The observed IR spectra is as shown in Fig. 1 and Fig.2. A broad band centered on 2970 cm^{-1} in the IR spectrum indicates the presence of a protonated carboxyl group and is assigned to an OH stretching. The down shifted stretching wave numbers is due to the presence of O-H...O hydrogen bonding.

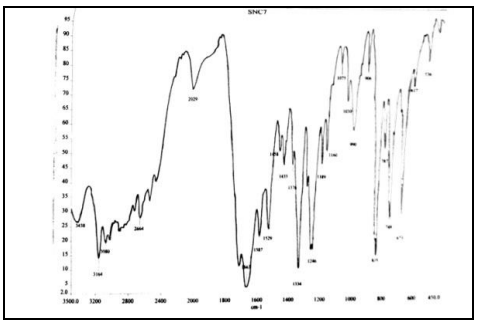

Figure 1. FTIR Vibrational Spectra (4000-450 cm^{-1})

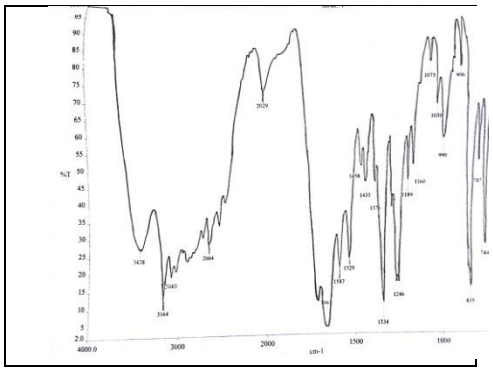

Figure 2. FTIR Vibrational Spectra (3500-450 cm^{-1})

The strong and broad peak at 1633cm^{-1} in the IR spectrum has been assigned to the carboxylate asymmetric stretching mode of the trichloroacetate anion. The symmetric stretching mode for IR is found at 1433 cm^{-1}.

The observed NH_3^+ group asymmetric stretching in IR is at 3164 cm^{-1} and 1663 cm^{-1} denotes asymmetric deformation. The C-S-C symmetric stretching mode is observed at 673 cm^{-1}. The C- O (H) stretching mode is observed as strong in the region 1189, 1140 cm^{-1}in IR spectrum.

IV. CONCLUSION

In the present study, single crystals of DL – Methionine with trichloroacetic were grown successfully using solution growth method. The FTIR spectra were recorded and complete vibrational assignments were made in order to identify the

presence of various functional groups of the grown sample. The results were compared with those of parent compounds and reported literature values. The result reveals that the molecules of the title compound are held together by hydrogen bonds in addition to van der waal's interactions. The downshifting of several stretching frequencies together with the increase in many of the deformation frequencies confirms the existence of extensive intermolecular hydrogen bonds in the structure.

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