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Structural Elucidation by Spectroscopic Studies of Copper (II) Groundnut Complexes with 2-amino-6-ethoxy benzothiazole as a Ligand

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Abstract:

Copper (II) soaps have a tendency of coordination with nitrogen and sulphur containing ligands. Synthesized copper (II) soap complexes may play an important part in pharmacological effects. In recent decades, the metal-ligand complexes with large-ring nitrogen and sulphur containing six-membered heterocyclic ligands have been an attractive and interesting area of scientific investigation in chemical research community worldwide. Copper (II) soap synthesized from groundnut oil and their complex formation with substituted benzothiazole ligand (i.e. 2-amino-6-ethoxy benzothiazole) has been described by spectral analysis. The method and condition of preparation of metallic soaps, have been widely studied to understand the characteristics and structure of these soaps.

Keywords — Copper soap, Metal-ligand complexes, Groundnut oil, Spectral analysis

I. INTRODUCTION

Surfactants are an important category of surface active compounds, which are derived from natural edible and non-edible oils and fats. Synthesis of metallic soaps from alkaline metals like sodium, potassium and ammonium represents metathesis reaction [1-2]. The metallic soaps are long-chain carboxylates of these metal ions. Metallic soaps are commercially significant owing to its uses in different applications like combustion aids, components of lubricating greases, cosmetic products, driers in inks or paints, heat stabilizers for plastics (particularly PVC) and water proofing agents [3-4].

Copper (II) soap complexes are being significant due to their toxicity in nature and their eco-friendly nature having antimycotic, weed control agent and many other bio-chemical activities. Groundnut oil provides an inexpensive source of high quality dietary protein and oil. Its major component fatty acids are oleic acid (58%) and linoleic acid (24%). The oil also contains some palmitic acid, arachidic acid, arachidonic acid, behenic acid, lignoic acid and other fatty acids. Due to the existence of larger number of ester bonds, the groundnut oil indicates high saponification value, signifying that the fat molecules were intact [5-7]. These properties formulate it valuable in soap production industry, it is not attractive as a unrefined substance as a consequence of its cost-effective and nutritive implications.

II. MATERIALS AND METHODS

Copper soap derived from edible oil such as groundnut and their complex formation with substituted benzothiazole ligand (i.e. 2-amino-6-ethoxy benzothiazole) have been characterized by spectral analysis.

LR/AR grade chemicals have been used in synthesis. Solvents such as benzene and ethanol have been purified before use by standard procedures.

Copper (II) soaps have been prepared by direct metathesis process. In this process, the oil has been refluxed with Potassium hydroxide solution and ethyl alcohol for about 3 hours. Hydrochloric acid has been used for neutralization of excess Potassium hydroxide. Essential amount of saturated solution of copper sulphate have been added with dynamic stirring [8]. The green precipitate has been procured. The copper soaps have been refined by recrystallization with hot benzene several times. The copper metal has been analyzed by standard procedure. These copper soaps were obtained in green colour.

III. RESULT AND DISCUSSION

In order to study the structure of Copper (II) groundnut soap complexes, the Infra-red spectra of complexes have been obtained from Department of chemistry, S.P.C. Govt. College, Ajmer on a ABB Horizon spectrophotometer instrument. The ESR spectra of copper (II) groundnut soap complexes have been recorded at liquid nitrogen temperature (LNT) from SAIF, IIT, POWAI, Mumbai using Tetracyanoethylene as a internal standard, whose g value is 2.00277. ^{1}H NMR spectra of copper (II) groundnut soap complexes have been recorded at CDRI, SAIF, Lucknow using Deuterated benzene as reference.

1. *INFRA-RED SPECTRAL ANALYSIS*

The absorption bands corresponds to asymmetric and symmetric stretching of methylene ($–CH_2$) group observed at 2924 and 2854 cm^{-1}. In the spectra of carboxylate ion (COO^-) two bands observed such as a strong asymmetrical stretching band in the range 1551-1558 cm^{-1} and a weaker symmetrical stretching band near 1373 cm^{-1}. Also >C=O stretching bands were observed at 1744 cm^{-1} [9-10].

A small band has been observed at 1234 cm^{-1} assigned to $–CH_2$ twisting and wagging vibrations. The band appears at 1157 cm^{-1} and 717 cm^{-1} corresponds to $–CH_3$ and $–CH_2$ rocking vibrations respectively. The band observed at 609 cm^{-1} may be assigned to copper–oxygen (Cu–O) stretching vibration.

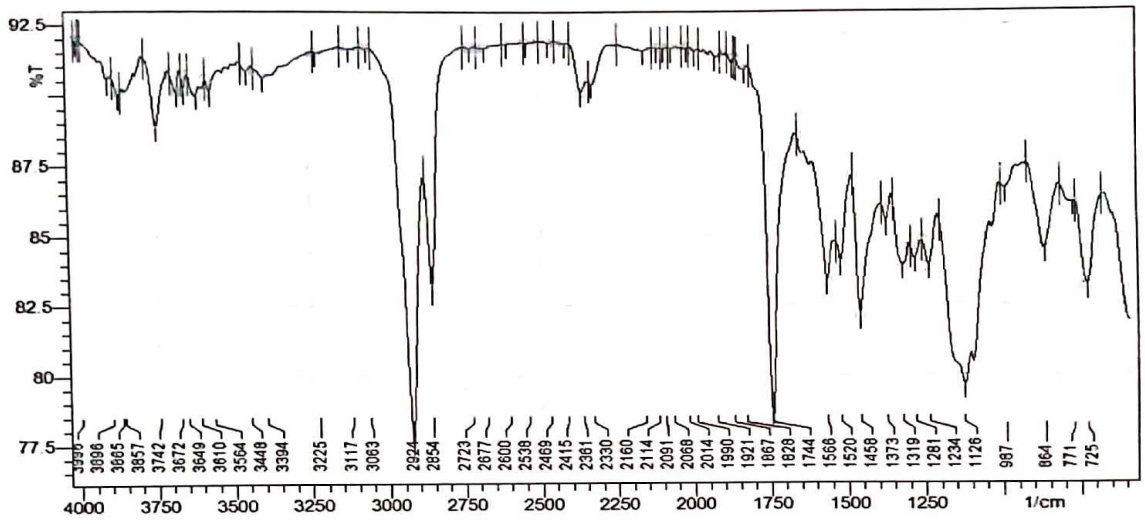

Fig. 1 IR spectra of copper (II) groundnut 2-amino-6-ethoxy benzothiazole complex (CGB_e).

NMR SPECTRAL ANALYSIS

Figure 2 shows NMR spectra of copper (II) groundnut 2-amino-6-ethoxy benzothiazole complex (CGB_e). Aliphatic $–CH_3$ and $–CH_2$ proton attached to $–CH_2R$ group show signal at nearly 0.957 δ and 1.290 δ respectively. The signal observed at 2.10 δ corresponds to $–CH_2$ proton attached to –C=C– group. Vinylic proton exhibits signal at 5.50 δ. A broadened peak is observed in the range δ 3.20 - 4.20 attributed to NH_2 group [11]. The appearance of this peak gives evidence of the coordination through the $–NH_2$ group of benzothiazole to the metal atom of the surfactant.

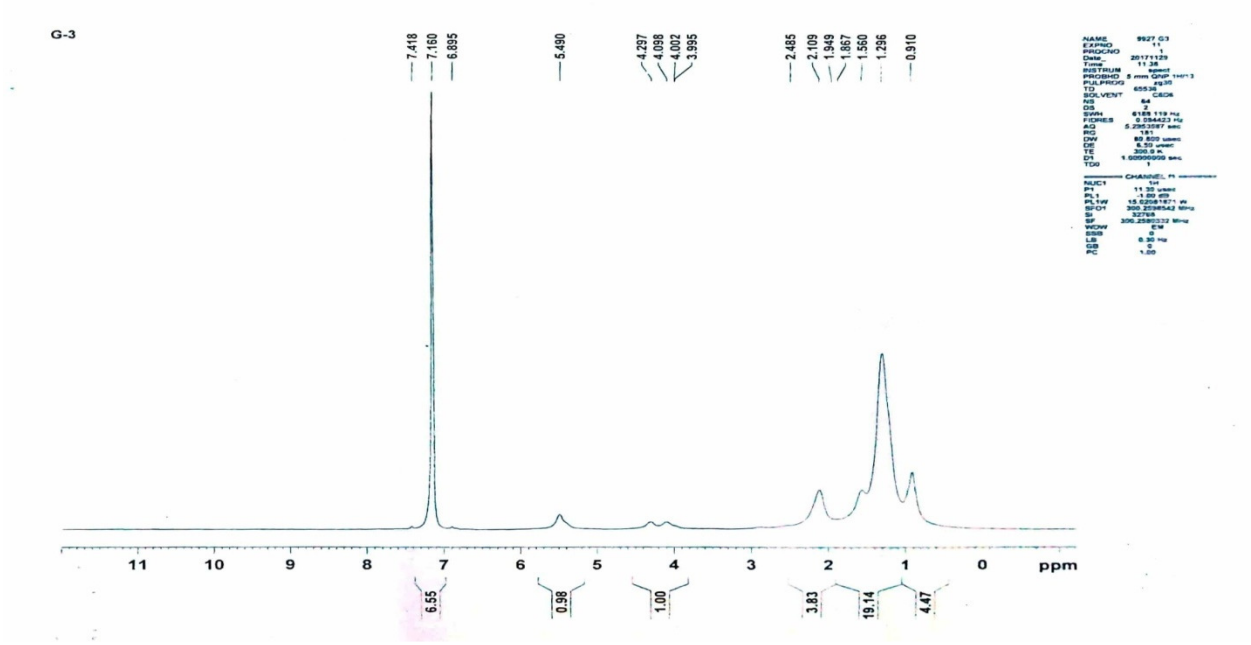

Fig. 2 NMR spectra of copper (II) groundnut 2-amino-6-ethoxy benzothiazole complex (CGB_e).

ESR SPECTRAL ANALYSIS

The Electron Magnetic Resonance (ESR) spectra of Cu (II) give information regarding the extent of the delocalization of odd electron. The ESR spectra of the copper (II) groundnut soap complexes have been archived on X-band at oscillation frequency of 100 KHz in the solid state at room temperature. Tetracyanoethylene (TCNE, g = 2.00277) has been used as the field marker and g_{II}, $g_{\perp}$, g_{av}, G values have been calculated. ESR spectra of the complexes exposed two g values (g_{II} and $g_{\perp}$). While the g_{II} and $g_{\perp}$ values are closer to 2, $g_{II} > g_{\perp}$ indicates a tetragonal distortion around the Cu (II) ion [12-13].

The pattern $g_{II} > g_{\perp} >$ ge (2.00277) indicates that the free (unpaired) electron is localized in dx^2-y^2 orbital in the lowest energy state of Cu (II), spectra are attributes axis of symmetry. This information assist that complexes have protracted octahedral shape. The $g_{II} > 2.3$ is a characteristic of an ionic environment and $g_{II} < 2.3$ indicates a covalent environment in the metal-ligand bonding. The g_{II} values for these complexes are less than 2.3 indicates that the environment is covalent [14-15].

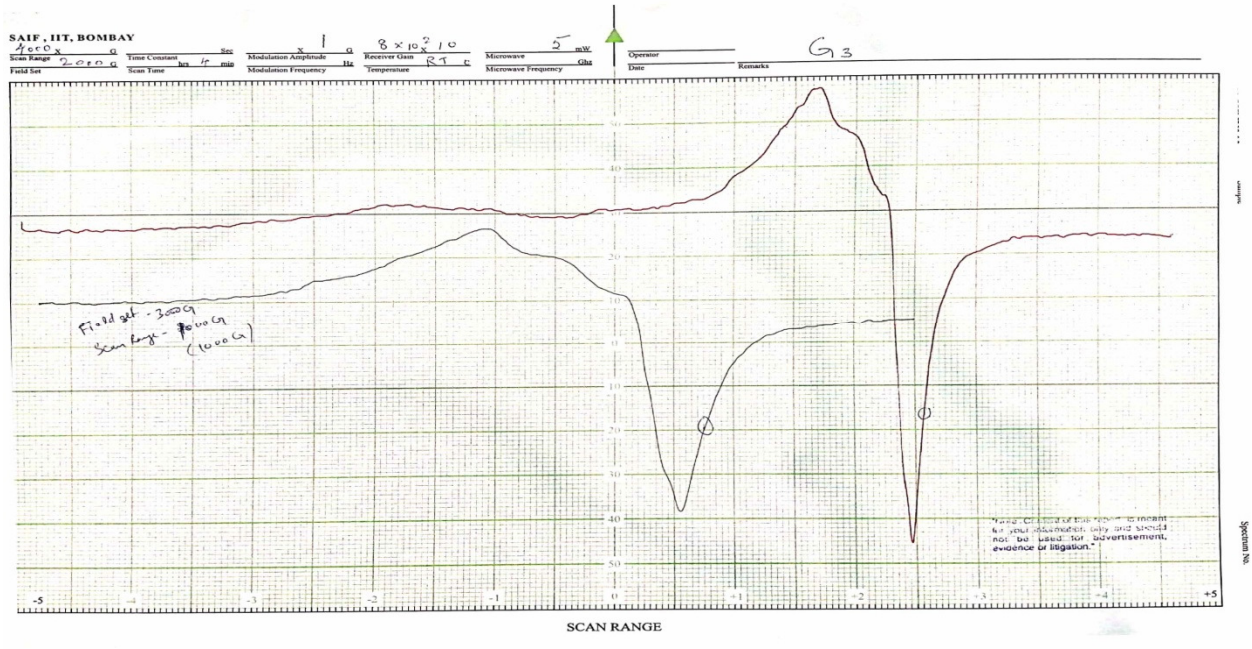

Fig. 3 ESR spectra of copper (II) groundnut 2-amino-6-ethoxy benzothiazole complex (CGB_e).

IV. CONCLUSION

The present research work shows relevant physicochemical mechanisms of these pharmaceutically important copper (II) soap complexes from natural edible oil such as groundnut. These pharmacologically interesting copper soap complexes could be a suitable strategy to develop novel therapeutic tools for the medical treatment.

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