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SYNTHESIS OF A COORDINATION COMPLEX BASED ON BENZENE-1,3,5-TRICARBOXYLIC ACID AND COPPER(II) ACETATE AND ITS IR SPECTROSCOPIC ANALYSIS

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Abstract: In the field of coordination chemistry, complexes based on polyfunctional ligands, especially aromatic compounds containing carboxyl groups, are increasingly gaining attention. In this study, a new coordination complex was synthesized through the reaction of benzene-1,3,5-tricarboxylate (BTC) ligand with copper(II) acetate in a 1:1 molar ratio. Under experimental conditions, an ethanol solution of BTC and an aqueous solution of Cu(II) salt were mixed and stirred with a magnetic stirrer at 60 °C for 1 hour, then left to crystallize at room temperature for one week. The resulting green crystalline substance was analyzed by infrared (IR) spectroscopy. The IR spectral results confirmed the formation of the complex. The spectrum clearly showed vibrational bands corresponding to the carboxylate groups' ν(C=O) and ν(C–O) stretching, as well as low-frequency vibrations attributed to the Cu–O bond.

Keywords: Coordination complex, BTC, copper(II) acetate, IR spectroscopy, carboxylate, MOF, 1,3,5-benzenetricarboxylate, crystallization.

Introduction

Recently, significant research has been conducted on the self-assembly of organic and inorganic molecules in the solid state, as this expands the possibilities for designing new solid materials with desired physical and chemical properties. One important approach involves using organic cations as templates to coordinate metal ions. Hydrogen bonding between the organic cation and the metal layer plays a crucial role in understanding the structure of organic-inorganic hybrid materials, influencing the arrangement and distance of adjacent metal layers or chains. Despite recent advances, predicting and controlling the supramolecular assembly of molecules remains challenging, and a deeper study of intermolecular forces that determine the packing patterns of molecules in the solid state is required.

In order to prepare new organic/inorganic composite solid materials, we synthesized complexes formed by the interaction of protonated benzene-1,3,5-tricarboxylic acid with copper(II) ions. In this complex, Cu(II) ions are coordinated through benzene-1,3,5-tricarboxylate ligands and stabilized via Cu–O bonds and hydrogen bonding between them. This article discusses the synthesis and structural characterization of these mononuclear and polymeric copper(II)-trimesate (benzene-1,3,5-tricarboxylate) complexes. In the field of coordination chemistry, polyfunctional ligands—particularly aromatic compounds containing carboxyl groups—are attracting increasing scientific interest. These compounds possess multiple donor atoms and are capable of forming coordination complexes with metal ions in various geometries and coordination modes. Benzene-1,3,5-tricarboxylic acid (BTC), a symmetric aromatic ligand containing three carboxylic acid (–COOH) groups, is widely used in modern applications such as metal-organic frameworks (MOFs), gas storage technologies, catalysis, and drug delivery systems.

In this study, a coordination complex was synthesized based on BTC and copper(II) acetate. As a result of the reaction, a green crystalline compound was obtained. The resulting complex was analyzed by IR spectroscopy, and the analysis confirmed that the carboxyl groups were coordinated to the copper(II) ions in the structure.

Experimental Method

To synthesize the coordination complex, 0.0210 g of benzene-1,3,5-tricarboxylic acid (BTC) was first dissolved in ethanol (C_2H_5OH). Simultaneously, 0.02 g of copper(II) acetate monohydrate ($Cu(CH_3COO)_2 \cdot H_2O$) was dissolved in distilled water in a separate container. Both solutions were prepared in 5 ml volumes.

During the experiment, the BTC solution and the copper(II) acetate solution were poured into a special reaction vessel and stirred intensively at 60 °C for 1 hour using a magnetic stirrer. After stirring, the solution was left undisturbed at room temperature for 7 days.As a result, a green crystalline compound formed at the bottom of the vessel. The obtained crystals were analyzed using infrared (IR) spectroscopy, and the structure of the coordination complex was confirmed by spectral analysis.

Results and Discussion

The resulting coordination complex was obtained as a green solid. The IR spectroscopic analysis provided the following results: The IR spectrum of the green complex compound was recorded in the range of 4000–400 cm^{-1} using a PerkinElmer Spectrum Two FT-IR spectrometer. The spectrum revealed the main absorption peaks associated with the functional groups of the ligand and the metal complex (Figure 1). A peak at 1701 cm^{-1} corresponds to the free C=O (carboxylic) group, indicating that some of the carboxyl groups were not involved in coordination. Peaks observed at 1589 cm^{-1} and 1456 cm^{-1} correspond to the asymmetric and symmetric stretching vibrations of the carboxylate anion, respectively, confirming that coordination occurred through the oxygen atoms of the ligand. In the region of 1100–1000 cm^{-1}, vibrational bands related to C–O and C–C bonds of the ligand were observed. Peaks at 892, 782, and 677 cm^{-1} correspond to the out-of-plane bending vibrations of the aromatic C–H bonds of the benzene ring. The most significant peaks were observed at 611 cm^{-1} and 529 cm^{-1}, which are assigned to the stretching vibrations of Cu–O bonds. These peaks serve as strong evidence for the formation of the coordination complex.

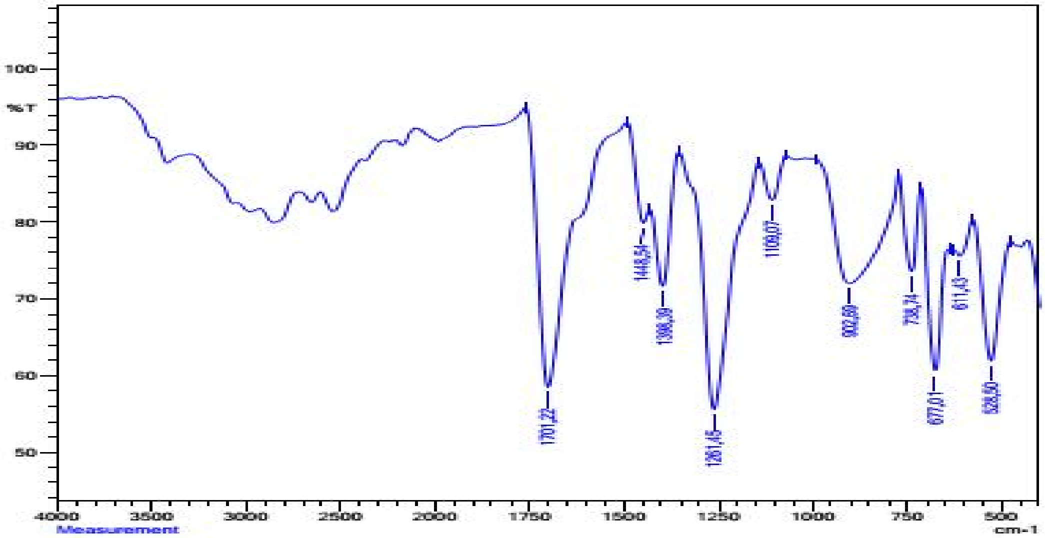

Figure 1.
IR spectrum of the synthesized copper(II)-BTC coordination complex.

Conclusion

A new coordination complex was synthesized based on benzene-1,3,5-tricarboxylic acid and copper(II) acetate. IR spectroscopic analysis confirmed that the carboxyl groups were coordinated to Cu^{2+} ions. Such complexes have the potential to serve as precursors for metal-organic frameworks (MOFs) and catalytic systems in future applications.

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