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SYNTHESIS AND ANALYSIS OF A COMPLEX COMPOUND BASED ON COBALT OXALATE AND SODIUM ACETATE

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Abstract

In this scientific study, a new Co(II)-oxalate-acetate complex compound was synthesized, and its physicochemical properties and structure were investigated using experimental and practical methods, and its composition was determined by infrared Functional groups and coordination bonds were identified using infrared (IR) spectroscopy. In addition, the compound's thermal stability, decomposition stages, and thermal properties were analyzed by thermogravimetric methods. The structure and energetic parameters of the complex compound were analyzed by quantum chemistry methods within the framework of DFT theory using the Gaussian 09 software. The theoretical results were found to be in good agreement with the experimental data.

Keywords: *Co(II) complex compound, oxalate and acetate ligands, infrared spectroscopy, thermal analysis, coordination compounds, DFT calculations; HOMO–LUMO*

Introduction

Today, the rapid growth of the population increases the demand for food, making it necessary to implement the achievements of chemistry, chemical technology, biology, medicine, and agricultural sciences into practice. In particular, the complex compounds formed between metals and organic ligands can serve as an example. Cobalt(II) ions, when coordinated with oxalate and acetate anions, form compounds with complex structures. The oxalate and acetate anions have multiple binding modes as ligands, through which various coordination environments can be created around the metal center. To synthesize such com-

pounds, a mixed-ligand complex compound containing Co(II) salts and oxalate acetate was prepared. The coordination properties of the oxalate ligand and its ability to bind to metal centers in mono- and bidentate modes have been demonstrated (Santana, 2020; Christensen, 2014). In these studies, the crystal structures of the complex compounds were investigated, and it was determined that the role of the oxalate ligand in the stability of the complex is significant. The thermal decomposition processes, stages, and thermal stability of oxalate-based complexes have been analyzed in detail (Lamprecht, Watkins, Brown, 2006). These results serve as an important scientific basis for the thermal analysis of oxalate complexes. Additionally, the multifunctionality of bimetallic complexes based on oxalate ligands, particularly their magnetic and electronic properties, has been extensively discussed (Clemente-León, Coronado, Martí-Gastaldo, Romero, 2011). Complexes containing acetate ligands, their interactions with metal ions, and coordination possibilities have been investigated (Seguel, Rivas, Paredes, 2010). The synthesis and characterization of complexes containing oxalate and acetate ligands have also been studied, and it has been investigated that the interaction between the ligands in such systems significantly affects the complex structure (Mishra, 2021; Al-Shehri, 2020). In particular, it has been shown that infrared (IR) spectroscopy can be used to identify metal–ligand bonds through the vibrational frequencies of functional groups (Tarasenko, 2018). This method is widely used to confirm the structure of complex compounds. A number of scientific papers on the synthesis and analysis of coordination compounds have also been carried out by local scientists. The synthesis of coordination compounds and their analytical methods have been systematically described (Nazarov, 2016), the physicochemical properties of cobalt-based complexes were studied (G'afurov, 2020), and the general properties and practical significance of organic ligand complexes were highlighted (Sharipova, Ibragimova, Khudoyberganov, Khallokov, Bobakulov, Abdullaeva, 2024). In recent years, research has extensively studied the synthesis of complexes based on acetate and other ligands with various metal ions. Recent studies have investigated the synthesis, structure, and properties of complex compounds based on divalent metal ions, including Co, Ni, and Cu, in the presence of acetate and other ligands. These results provide an important scientific basis for a deeper study of cobalt-based complexes. The literature review above shows that, the synthesis, structure, and properties of complexes containing oxalate and acetate ligands are a current scientific focus, and their in-depth analysis, especially using methods such as thermal analysis and infrared spectroscopy, is of great importance.

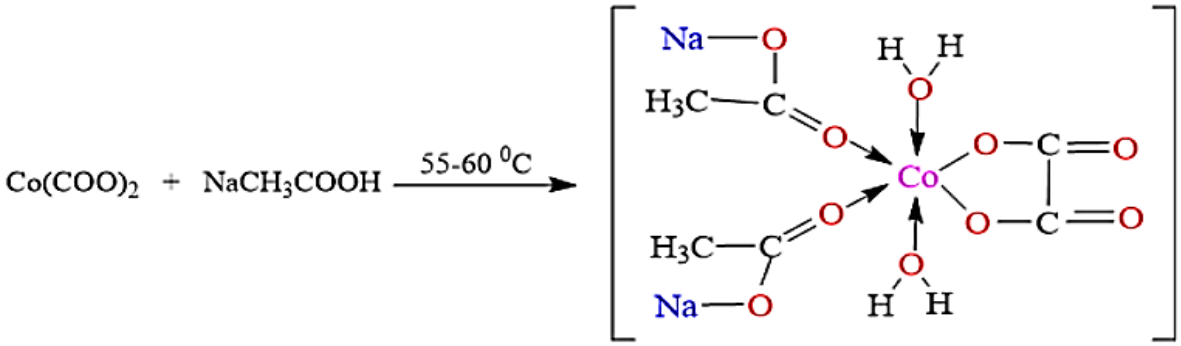
Research method

The following substances were used for the synthesis of the complex compound: cobalt chloride, oxalic acid, sodium hydroxide, and sodium acetate. The synthesis of the starting materials was carried out using the following method: a concentrated solution of the metal salt and an alkaline solution of the same concentration were combined to precipitate the metal hydroxide. The precipitate was washed five times by decantation, and an oxalic acid solution was poured over it. As a result, the metal's oxalate salt was formed.

$$CoCl_2 + 2NaOH = Co(OH)_2\downarrow + 2NaCl$$
$$Co(OH)_2 + (COOH)_2 = Co(COO)_2 + 2H_2O$$

The synthesis of the Co(II) oxalate–sodium acetate complex was carried out by the following method: 0.01 mol of Co(II) oxalate was dissolved in 10 ml of water. In another beaker, 0.02 mol of sodium acetate was dissolved in 15 ml of water by heating in a hot water bath (45–50 °C). Then, the sodium acetate solution was added dropwise to the Co(II) oxalate solution, and the mixture was stirred in a magnetic stirrer at 55–60 °C at 800 rpm for 1.5 hours. The resulting solution was left at room temperature for 72 hours to crystallize. As a result, colored complex compound crystals formed.

As a result of the solvent's slow evaporation, a dark-colored polycrystalline product was obtained. The product was filtered, washed with acetoneitrile, and dried at room temperature.



Results analysis

An elemental analysis was performed to determine the composition of the obtained compound (Table 1).

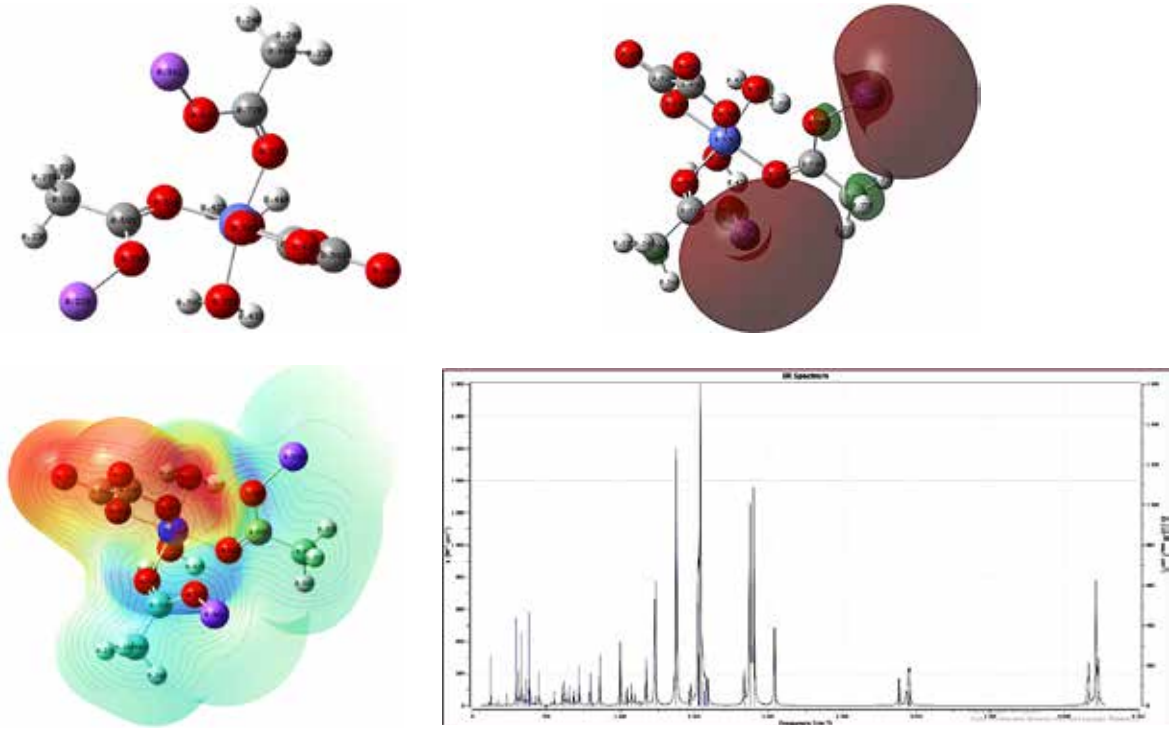
Table 1. *Results of the elemental analysis of the obtained complex compound*

Compounds		$[Co(CO_2)_2 \cdot 2CH_3COONa \cdot 2H_2O]$
Co	Calculated	17.10
	Determined	17.21
Na	Calculated	13.33
	Determined	13.21
C	Calculated	20.86
	Determined	20.88
O	Calculated	45.37
	Determined	45.42
Compound color		Dark pink
Reaction yield, %		89.15

Based on quantum chemical calculation results, the optimized geometric structure of the complex compound formed from Co(II) oxalate and sodium acetate is presented. The atoms in the molecule are represented by partial charges, and a redistribution of electron density around the central atom is observed. This is explained by the transfer of electron density to the metal center via the donor atoms of the ligands. As a result, donor–acceptor interactions arise in the complex, confirming the occurrence of electron flow (Figure 1).

The HOMO orbital is primarily localized around the oxygen atoms in the ligands, indicating their high electron density. The LUMO orbital is partially located on the central cobalt atom and its surrounding coordination environment. This distribution indicates that the electron transfer in the complex is primarily from the ligands to the metal center, favoring a ligand-to-metal charge transfer (LMCT) mechanism. The electrostatic potential distribution (ESP) of the molecule is shown in the figure. In it, the red color represents regions with high electron density (electron donor centers), while the blue color represents regions with low electron density (electron acceptor centers). According to the analysis results, the largest negative potential is mainly concentrated around the oxygen atoms, which manifest as active donor centers. The largest positive potential is observed around the central cobalt atom. In particular, the dense contours between the cobalt atom and the coordinated oxygen donor atoms confirm the strength of the coordination bonds. The experimental IR spectrum of the synthesized Co(II)–oxalate–acetate complex was compared with the theoretically calculated spectrum. During the comparison, the absorption frequencies, shifts, and intensities of the main functional groups were analyzed.

Figure 1. *Mulliken method – derived electron charge distribution of the complex compound formed from Co(II) oxalate and sodium acetate (a), View of molecular orbitals (HOMO and LUMO) (b), Distribution of the molecular electrostatic potential (MEP) and the complex's complete energy spectrum (distribution of orbital energies) (c), Theoretically calculated IR spectrum of the complex compound based on cobalt oxalate and sodium acetate by quantum chemical methods (d)*



In the practical IR spectrum, the strong absorption peaks observed in the 1600–1650 cm^{-1} and 1350–1450 cm^{-1} ranges correspond to the asymmetric (vas) and symmetric (vs) vibrations of the $–COO^-$ group, respectively. These peaks appear in the theoretical spectrum in almost the same regions, confirming the presence of cobalt oxalate and sodium acetate ligands in the complex. In the experimental spectrum, the difference between the vas and vs vibrations (Δν) indicates the alignment of the carboxylate groups with the Co(II) center. This situation allows for the assumption that the oxalate ligand is bidentate, while the acetate ligand is monodentate or bridging. The small shifts (10–40 cm^{-1}) between the theoretical and experimental IR spectra are attributed to experimental conditions (solid phase, crystal lattice effect), hydrogens, the actual coordination environment of the ligands, and the assumption of ideal conditions in the computational method. Nevertheless, a high degree of agreement was observed in the positions and intensities of the main absorption peaks. The comparison of experimental and theoretical spectra demonstrated the successful synthesis of the Co(II)–oxalate–acetate complex.

Table 2.

ν_{exp} (cm^{-1})	ν_{calc} (cm^{-1})	Type of vibration	Analysis
3200–3500	3300–3450	ν(O–H)	Water or hydrogen bonding
1600–1650	1580–1620	$\nu_{as}(COO^-)$	Asymmetric vibration of the carboxylate group in oxalate and acetate

ν_{exp} (cm^{-1})	ν_{calc} (cm^{-1})	Type of vibration	Analysis
1350–1450	1360–1420	$\nu_s(COO^-)$	Symmetric vibration of the carboxylate group
1000–1300	1020–1280	ν(C–O), ν(C–C)	Ligand backbone vibrations
400–600	420–580	ν(Co–O)	Metal–oxygen coordination bonds

As can be seen from the table, the difference between the experimental and theoretical values is not large (±10–40 cm^{-1}), which confirms the successful synthesis of the Co(II)–oxalate–acetate complex compound by comparing the experimental and theoretically calculated IR spectra. In this work, the thermal properties of the synthesized Co(II) oxalatacetate complex compounds were investigated using TG, DTA, and DSC methods, which provided details on the compounds' thermal decomposition stages and energetic changes. The thermal analysis of the cobalt oxalate–sodium acetate complex compound was studied based on TGA and DTA curves. According to the analysis results, multiple decomposition stages were observed as the compound was heated. Initially, a weight loss of approximately 17.9% was recorded in the temperature range of 30–145 °C, which is associated with the desorption of adsorbed or crystallized water molecules within the complex. This process is confirmed by an endothermic peak observed on the DTA curve at approximately 112.95 °C, which indicates the presence of hydrogen bonds in the complex.

Conclusion

Based on the structures of the initial compounds, analyses were conducted to determine their molar ratios. These analyses assessed reactivity through the difference between the HOMO and LUMO (ΔE) and determined which compound is more reactive or more stable. IR spectroscopic analysis proved that the coordination compounds formed in the interaction of metal acetates with Co(II) oxalate are heterometallic complexes, and that the coordination bond is formed through the bidentate bridging coordination of the acetate groups. The results of the thermal analysis, namely the disappearance of the characteristic reflections of the starting materials and the appearance of new peaks, reliably confirm the formation of the complex compound and its existence in a separate crystalline phase. The results of this analysis confirm the presence of crystallization water molecules in the $[Co(CO_2)_2 \cdot 2CH_3COONa \cdot 2H_2O]$ complex compound and the stepwise decomposition of the ligands.

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