ISNN 3030-3907

2026
MAY
ISSUE - 5
VOLUME - 6

DEVELOPMENT OF SCIENCE

scientific journal



Development of science

Ilmiy jurnal

MAY 2026
Issue - 5, VOLUME – 6

ISSN 3030 -3907

Ilmiy jurnal OAK rayosatining 2024 yil 27 sentabrdagi 361-son qaroriga asosan 02.00.00 kimyo fanlari hamda 2025 yil 12 fevral 367- son qaroriga asosan 05.00.00 texnika fanlari bo‘yicha falsafa doktori (PhD) va fan doktori (DSc) ilmiy darajasiga talabgorlarning dissertatsiya ishlari yuzasidan dissertatsiyalari asosiy ilmiy natijalarini chop etish tavsiya etilgan milliy ilmiy nashrlar ro‘yxatiga kiritilgan.

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ISSN 3030-3907

UDK: 546.73 + 547.79 + 547.562:544.478

SYNTHESIS AND ANALYSIS OF A Co^{2+} BASED COORDINATION COMPOUND WITH CEFOTAXIME AND ACETAMIDE LIGANDS

Azamat Masharipov

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Annotatsiya. Kobalt (II) xlorid, sefotaksim va atsetamid ishtirokida aralash ligandli koordinatsion kompleks sintez qilinib, uning tarkibiy tuzilishi elementar tahlil orqali aniqlashtirildi. Olingan birikmalarning fazoviy konfiguratsiyasi hamda energetik ko‘rsatkichlarini chuqurroq anglash maqsadida kvant-kimyoviy hisoblashlar amalga oshirildi. Kompleks tarkibida metall markaz va ligandlar o‘rtasidagi o‘zaro bog‘lanishning molyar nisbatlari aniqlanib, ularning muvofiqlashuv xususiyatlari yoritildi.

Kalit so‘zlar: koordinatsion kompleks, sefotaksim, asetamid, SEM–EDX tahlil, kvant-kimyoviy modellashtirish.

Аннотация. Синтезирован смешаннолигандный координационный комплекс с участием хлорида кобальта (II), цефотаксима и ацетамида, его элементный состав и структура были уточнены методом элементного анализа. Для более глубокого понимания пространственной конфигурации и энергетических показателей полученных соединений были проведены квантово-химические расчеты. Определены молярные соотношения между металлическим центром и лигандами в составе комплекса и описаны их координационные свойства.

Ключевые слова: координационный комплекс, цефотаксим, ацетамид, СЭМ-ЭДС анализ, квантово-химическое моделирование.

Abstract. A mixed-ligand coordination complex involving cobalt (II) chloride, cefotaxime, and acetamide was synthesized, and its elemental composition was determined through elemental analysis. Quantum-chemical calculations were performed to gain a deeper understanding of the spatial configuration and energetic parameters of the resulting compound. The molar ratios of the interaction between the metal center and the ligands within the complex were determined, and their coordination characteristics were elucidated.

Keywords: coordination complex, cefotaxime, acetamide, SEM–EDX analysis, quantum-chemical modeling.

INTRODUCTION.

Coordination chemistry, a key branch of modern inorganic and bioinorganic chemistry, is based on the study of interaction mechanisms between metal ions and ligands of various natures. Such complex compounds are

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noteworthy not only from a theoretical standpoint but also for their practical significance, particularly their wide application in fields such as pharmaceuticals, catalysis, and materials science.

In recent years, the synthesis of metal complexes based on biologically active substances has become one of the most pertinent areas of scientific research. In particular, when antibiotics form complexes with metal ions, a significant change or increase in their biological activity is observed. β-lactam antibiotics, such as cefotaxime, can coordinate with metal ions to form complexes with novel properties.

LITERATURE REVIEW.

The cobalt (II) ion is one of the most widely studied metal centers in coordination chemistry and possesses the ability to form stable complexes with ligands having various donor atoms. Co (II) complexes typically exist in various geometries (octahedral, square-planar), and their structure is directly dependent on the nature of the ligand [1].

Furthermore, amide-type ligands, particularly acetamide, play a crucial role in coordination with metal ions. The ability of such ligands to bind to the metal center through O and N donor atoms to form stable complexes is considered important for bioinorganic chemistry [2-3].

Therefore, the synthesis of mixed-ligand complexes that unite ligands with different functional groups around a single metal center and the study of their properties are of great scientific and practical importance [4-6]. The aim of this work was to synthesize a mixed-ligand coordination compound based on cobalt (II) chloride, cefotaxime, and acetamide, and to determine its composition, structure, and energetic properties.

In coordination chemistry, mixed-ligand complexes hold a special place, as they acquire new physicochemical and biological properties resulting from the interaction of different ligands. Studies in the literature indicate that transition metals, including Co (II), form strong coordination bonds with ligands containing various donor atoms, and these complexes often exhibit high stability [7-11].

Metal complexes derived from biologically active ligands are of particular interest. Specifically, metal complexes synthesized from cefotaxime and other antibiotics have been found to possess antibacterial, antioxidant, and even antitumor properties [12]. This suggests that the efficacy of medicinal substances can be enhanced through metal complexation.

Furthermore, there are studies on the coordination of cefotaxime with various metal ions, which show that the resulting complexes have been characterized using IR, UV-Vis, and thermal analysis methods [13-17]. These

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works are of great importance for determining the mechanisms of ligand-metal bonding.

Carboxamide ligands, such as acetamide, are common in coordination chemistry and form various coordination modes with metal ions. Such complexes play a significant role in bioinorganic processes, particularly in enzyme models and catalytic systems [18].

Furthermore, complexes derived from various organic ligands with Co (II) ions have been extensively studied using elemental analysis, IR spectroscopy, and thermal analysis methods [19]. This highlights the necessity of a comprehensive approach for determining the composition and structure of synthesized complexes.

In recent studies, quantum-chemical calculation methods have been widely applied to determine the spatial structure of mixed-ligand complexes. These methods enable the determination of the energy stability, geometry, and electronic structure of the complexes [20].

The literature review above indicates that mixed-ligand complexes based on cobalt (II), cefotaxime, and acetamide have not yet been sufficiently studied in depth, making their synthesis and comprehensive analysis a scientifically pressing issue.

RESEARCH METHODOLOGY.

It is well known that quantum chemistry, with its extensive computational results, good experimental data, and in-depth approaches, is currently considered a high-level method for solving biochemical, materials science, and other fundamental and applied problems. Quantum chemical methods not only allow for the calculation of the properties of individual molecular systems but also enable the identification of general regularities characteristic of selected classes of molecules and the substantiation of existing laws in chemistry. Furthermore, by studying their influence on and dependence on general regularities, these methods make it possible to determine the basis for establishing these relationships. Based on quantum-chemical calculation methods, it is possible to predict the competitive donor centers of multifunctional ligands that will undergo coordination.

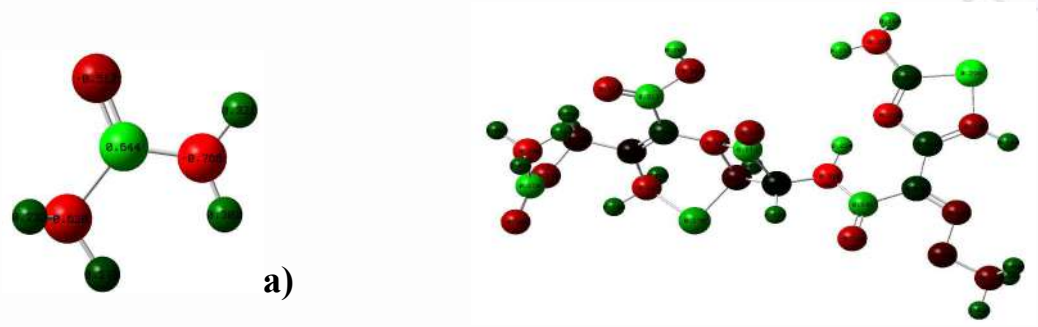
Due to the high propensity of ligands containing a carbonyl group to form coordination compounds, various complex compounds have been synthesized, and their compositions and properties studied. If O- and N-containing ligands, including amides, are introduced into compounds with such properties, studying their formation of complex compounds together is of theoretical and practical importance. This is because ethanolamines possess high reactivity, exhibiting

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both amine and alcohol properties. As a result of their ability to form various denticities, it is possible to synthesize mixed-ligand complex compounds.

Various physicochemical properties of cefotaxime and acetamide were analyzed using quantum-chemical methods with the Gaussian 09 software package. The calculations were performed using the B3LYP method within the framework of DFT theory. The HyperChem and GausView programs were used to create and visualize the model systems [1-3].

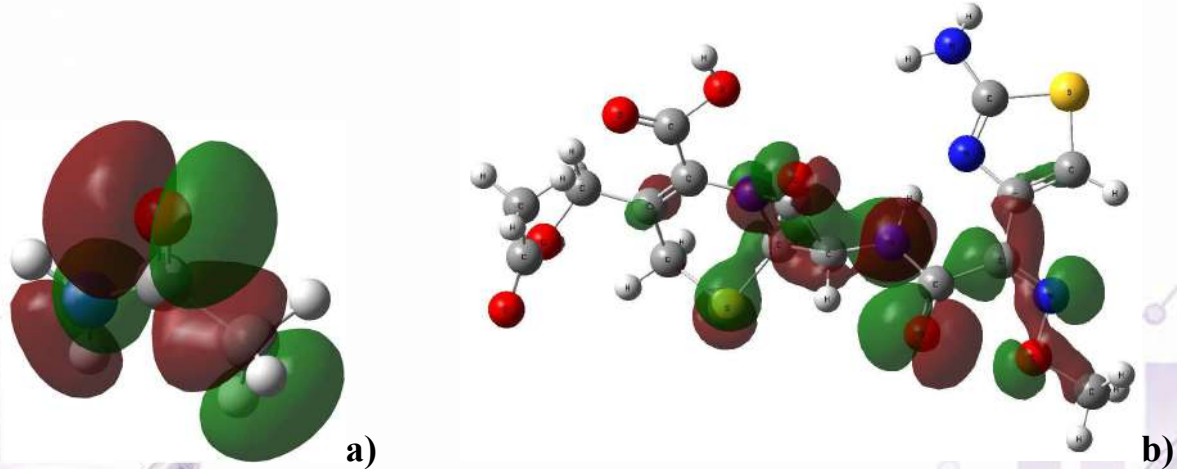
In the initial stage of the theoretical research, the system was optimized. In the next stage, the main calculations were carried out. Figure 1 shows the optimized electronic structure of the ligands and the distribution of Mulliken charges within them.



a) b)

Figure 1. The optimized electronic structure of the ligands and the distribution of Mulliken charges therein: acetamide (a), cefotaxime (b)

Furthermore, within the scope of the quantum-chemical calculations, the state of the electron orbitals of the ligand molecules in the ground state (HOMO) and the excited state (LUMO) was investigated. The results of the calculations are presented in Figure 2.

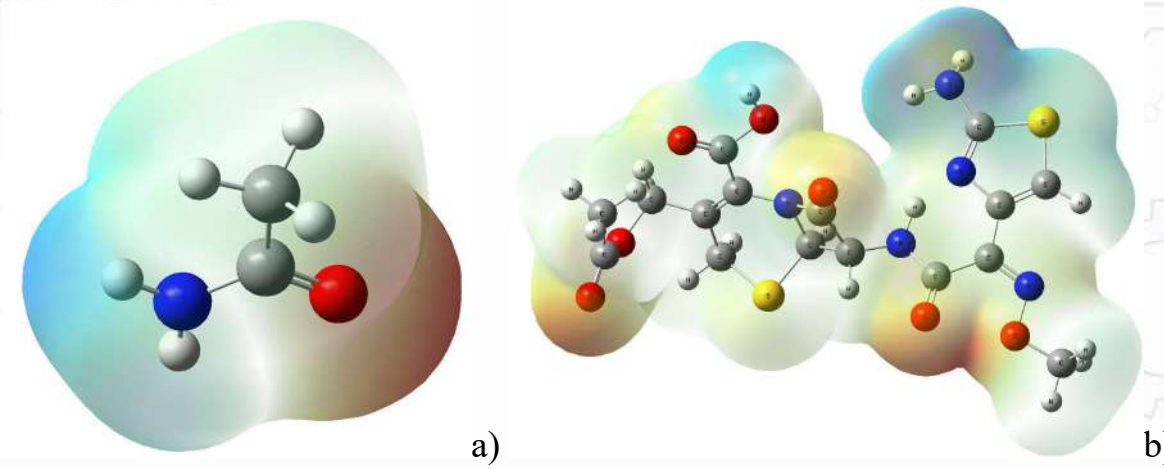


a) b)

Figure 2. The state of the electron orbitals of acetamide and cefotaxime molecules in the ground and excited states

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The calculations show that the energy gap between the ground state (HOMO) and the excited state (LUMO) is 2.232 eV for acetamide and 3.199 eV for cefotaxime.



a) b)

Figure 3. Geometric structure and MEP distribution of acetamide (a) and cefotaxime (b) molecules

The red and blue regions of the MEP (molecular electrostatic potential) maps represent negative and positive electrostatic potentials, respectively. In the color scheme of the MEP map, the red region indicates atoms with a lone electron pair or a negative electrostatic potential; the intensity of the color is proportional to the absolute value of the potential energy. Positive electrostatic potentials are shown in the blue/yellow regions and characterize the polar hydrogen in E–N bonds. Green areas cover parts of the molecule where the electrostatic potential is close to zero (C–C, C–N).

The energetic, geometric, and electronic properties of the ligand molecules were calculated. The bond angle and bond length values of the ligands were determined. Quantum-chemical studies involve several successive stages, such as constructing a model, optimizing it, performing spectroscopic and thermodifferential calculations, and processing and visualizing the results.

Quantum-chemical calculations were conducted to determine the possible coordination centers, coordination capabilities, and energetic, geometric, and electronic parameters of the ligand molecule. Based on the results of these calculations, the ligands were identified by their minimum energy of formation. The low energy of formation for the ligand molecules indicates their stability.

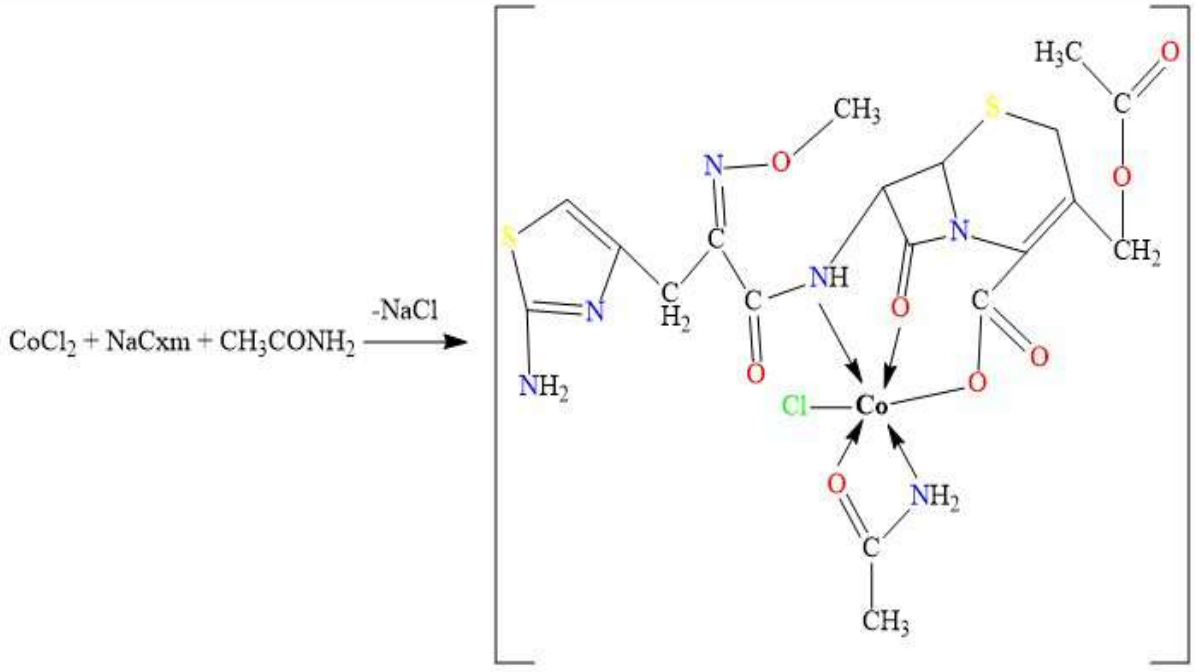
Based on the magnitude of the charges on the donor atoms of the ligands, it is evident that the highest negative effective charge in the molecule is located on the oxygen atom of the carbonyl group and on the nitrogen atom of the amino group.

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Based on the values of electron densities and effective charges on the donor and reaction-active atoms of the ligand molecules, the results obtained were found to be consistent with data from the literature.

It follows that in the molecules of potentially tetra-, penta-, and hexadentate ligands, complex formation can occur through coordination via the oxygen atom of the carbonyl group and the nitrogen atom of the amino group. In this case, because these two centers of high negativity are located on opposite sides of the molecule, they can either form a polynuclear complex, acting as a bridge between two metal ions, or the atoms on only one side (C=O or H_2N-C) can coordinate in a bidentate manner.

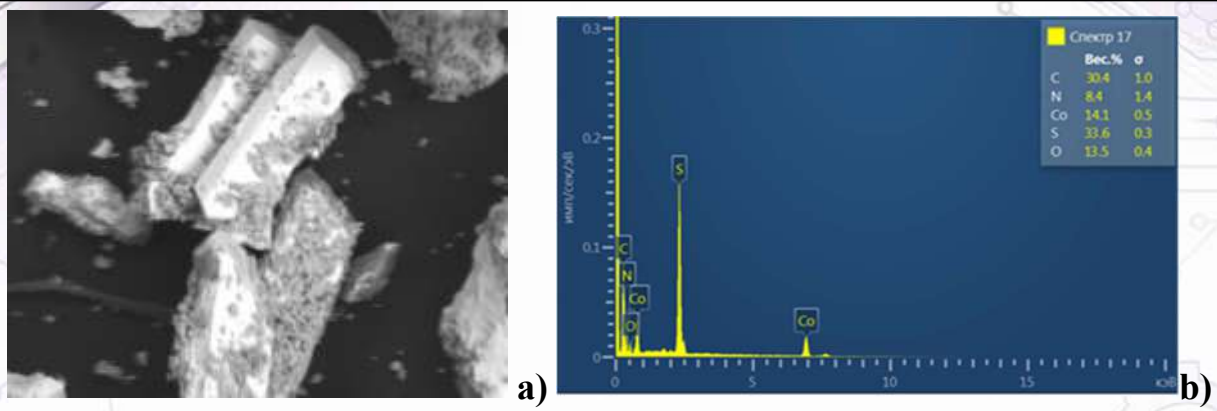
Based on the obtained quantum chemical results, it was determined that a 1:1:1 ratio provided the optimal conditions for synthesizing the mixed-ligand complex compound. The following method was employed: aqueous, acetonitrile, and aqueous solutions of $CoCl_2$ (0.001 mol), cefotaxime (0.001 mol), and acetamide (0.001 mol), respectively, were mixed for 1.5 hours at 40°C using a magnetic stirrer at 800 rpm. A dark red solution was obtained as a result [11]. This solution was left at room temperature for 12 days until crystals formed.



ANALYSIS AND RESULTS.

To compare with the theoretically calculated elemental quantities in the obtained mixed-ligand coordination compound, elemental analysis of the complex compound resulting from the reaction was performed using scanning electron microscopy–energy dispersive X-ray spectroscopy (SEM-EDX), and their quantities were found to be consistent (Figure 4).

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a) b)

Figure 4. Microstructure (a) and EDX result (b) of [$CoC_{17}H_{20}N_7O_8S_2Cl$]

According to the SEM-EDT results, numerous peaks characteristic of the metal ion were recorded, along with the formation of a complex with the metal ion and a change in the ligand's microstructure. The degree of crystallinity of the new complex compound was also determined. By comparing the results of the quantum chemical analysis with the data obtained from the SEM-EDT analysis, it was determined that a coordination number of 6 for cobalt corresponds to the structure with the minimum energy (Fig. 5).

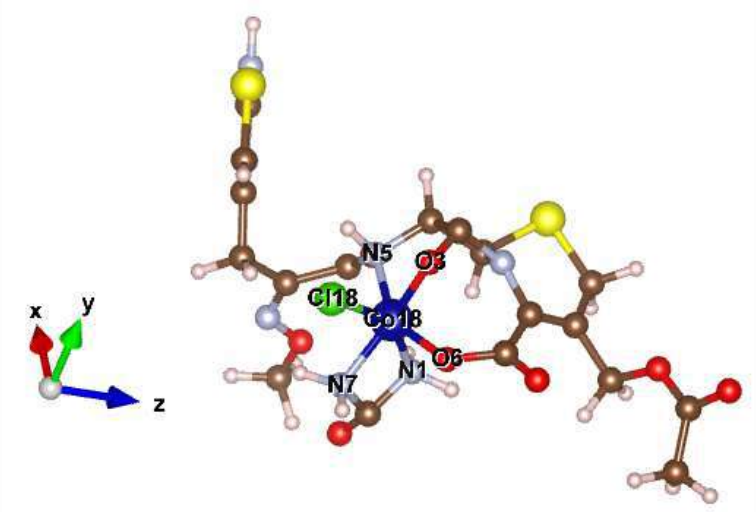


Figure 5. Spatial structure of the [$CoC_{17}H_{20}N_7O_8S_2Cl$] compound.

CONCLUSION.

A mixed-ligand complex compound of cobalt (II) chloride with cefotaxime and urea was synthesized. SEM-EDT and quantum chemical calculations were performed to prove the formation of a coordination bond in the newly synthesized compound. Based on the results obtained, it was determined that in the [$CoC_{17}H_{20}N_7O_8S_2Cl$] compound, cobalt forms ionic bonds through the oxygen of the carboxyl group anion of the cefotaxime ligand and through the chloride anion. It also forms coordination bonds with the nitrogen atoms of the four-membered heterocycle's carbonyl and the amide bond, as well as with the nitrogen atom of the amino group in the urea ligand, resulting in a coordination number of 6.

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