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SYNTHESIS, STRUCTURE AND ELECTRONIC PROPERTIES OF A NEW $[Zn(IAA)_2(AA)_2]\cdot 2H_2O$ COORDINATION COMPLEX: A COMBINED EXPERIMENTAL AND COMPUTATIONAL STUDY

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INTRODUCTION. One of the priority directions of modern coordination chemistry is the synthesis of new complex compounds of transition metals based on biologically active ligands and the fundamental study of their properties. Among transition metals, zinc (Zn(II)) stands out due to its low toxicity, its important role in biological processes, and its versatile coordination capabilities. Zinc ions are components of many enzymes and participate in regulating metabolic processes in the organism. In this study, indole-3-acetic acid (IAA), selected as a ligand, is one of the most important natural plant growth regulators (belonging to the auxin group). Due to the presence of donor atoms in its structure (the nitrogen in the indole ring and the oxygen in the carboxyl group), IAA is capable of forming stable and biologically active complexes with metal ions. The second ligand, acetamide, is a simple yet effective amide that exhibits high selectivity in coordination with d-metals and is frequently found in pharmaceutical compounds. The synthesis of mixed-ligand complexes is relevant not only for obtaining new substances but also from the perspective of studying intermolecular interactions. The investigation of the structure and properties of complex compounds formed by the simultaneous coordination of both a hormonal ligand (IAA) and an amido ligand around a zinc ion opens new prospects for agriculture and pharmaceutical applications. Modern chemical research is inconceivable without quantum-chemical analysis. The initially selected main ligand, indole-3-acetic acid (heteroauxin, IAA), and the newly synthesized coordination compound $[Zn(IAA)_2(AA)_2]\cdot 2H_2O$ were studied using the Gaussian program with the CAM-B3LYP basis set. The aim of this article is to synthesize a mixed-ligand complex compound of the Zn(II) ion with indole-3-acetic acid and acetamide, to confirm its composition using modern physicochemical methods, and to theoretically substantiate the stable structure and electronic properties of the complex through quantum-chemical calculations.

LITERATURE REVIEW AND METHODS. In recent years, the synthesis of metal complexes based on drugs and biologically active substances has remained one of the priority directions of coordination chemistry. In particular, compounds of Zn(II) ions with plant growth stimulators and heterocyclic ligands have been widely studied due to their biological effectiveness and low toxicity. Indole-3-acetic acid (IAA) is known as a plant phytohormone, and its coordination with metals significantly alters the biological activity of the molecule. In studies conducted by K. Szmigiel-Bakalarz and co-authors (2020), a new 2D coordination polymer of Zn(II) ions with IAA, $[Zn(I3AA)_2]n$, was synthesized [1]. The study showed that coordination occurs through the carboxylate group of the ligand, and the resulting complex exhibits higher microbiological activity compared to the free ligand.

Similarly, Xuling Xue and co-authors (2011) studied mixed-ligand complexes of IAA with auxiliary ligands such as 1,10-phenanthroline and 4,4'-bipyridine. Their results indicate that such complexes exhibit not only biological activity but also luminescent properties and can serve as sensors for mercury(II) ions. Complexes of Zn(II) ions with nitrogen- and oxygen-donor ligands are widely used in medicine [2,3]. In the studies of Qingdi Zhou (2000) and G.G. Nnabuike (2020), the synthesis of Zn(II) complexes based on indomethacin (a drug structurally similar to IAA) and nitrogen-donor ligands (pyridine, imidazole) was reported [6,11]. These works demonstrated that the gastrointestinal toxicity of zinc complexes is lower than that of Cu(II) complexes, and their pharmacokinetic properties are improved.

The synthesis of Zn(II) complexes with acetamide and its derivatives (such as aryl-acetamides) is also of current importance. Kishwar Sultana and co-authors (2016) synthesized zinc complexes based on aryl-acetamides and evaluated their potential as enzyme inhibitors and anticancer agents [8]. In the evaluation of the electronic structure and stability of coordination compounds, density functional theory (DFT) has become an indispensable method. In their studies, Ayesha Zahoor (2021) and Richa and co-authors (2020) calculated the geometric parameters, HOMO–LUMO energy gap, and molecular electrostatic potential (MEP) of Zn(II) carboxylate complexes using the DFT method [5,7]. Quantum-chemical calculations serve as a key tool in explaining through which centers synthesized complexes are coordinated and how their chemical reactivity is determined. For example, DFT studies performed by Karolina Babijczuk (2023) on zinc–indole–imidazole complexes theoretically confirmed that coordination enhances the functionality of biologically active ligands [4]. DFT analysis, along with global reactivity descriptors and thermal stability (TGA/DSC), has also been applied to dehydroacetate acid complexes [9]. For Zn(II)–Schiff base complexes, electronic parameters were calculated using DFT, demonstrating structural stability, and their interaction with DNA was analyzed using viscometry and UV/fluorescence methods [10]. The literature review shows that the synthesis of mixed-ligand complexes of Zn(II) ions with indole-3-acetic acid and acetamide derivatives, as well as the study of their structure using quantum-chemical methods:

1. Obtaining new biologically active substances;
2. Determining the coordination between the ligand and the metal;
3. Predicting the stability and reactivity of the compound.

The mixed-ligand coordination compound of zinc(II) chloride with indole-3-acetic acid and acetamide was synthesized using the following procedure. First, 0.01 mol (1.75 g) of indole-3-acetic acid (IAA) was dissolved in 50 mL of ethanol. To ensure deprotonation of the ligand's carboxyl group, 0.01 mol of potassium hydroxide (KOH) was added

to the resulting solution. In a separate beaker, 0.005 mol (0.85 g) of zinc(II) chloride dihydrate ($ZnCl_2 \cdot 2H_2O$) was completely dissolved in 20 mL of distilled water. The metal salt solution was then added dropwise to the indole-3-acetic acid solution under constant stirring and mixed on a magnetic stirrer for 25–30 minutes. Afterwards, in order to form the mixed-ligand complex, a solution of 0.01 mol (0.59 g) of acetamide (AA) was added dropwise (5–10 mL) to the reaction mixture, followed by further stirring for 25–30 minutes. The reaction mixture was then continuously stirred at 50–55 °C for 1–1.5 hours using a magnetic stirrer [12]. At the end of the reaction, a clear, colorless solution was obtained. The resulting solution was purified by filtration, washed several times with a mixture of distilled water and ethanol, and dried in a vacuum desiccator (over P_2O_5) until constant mass was achieved [13,14].

As a result of the synthesis process, a clear colorless crystalline powder was obtained. The overall yield of the synthesis reaction was 82%, which confirms the high efficiency of the selected synthetic method. Based on the compositional analysis of the complex compound, it can be represented by the formula $[Zn(IAA)_2(AA)_2] \cdot 2H_2O$ [15]. The reaction equation can be expressed as follows.

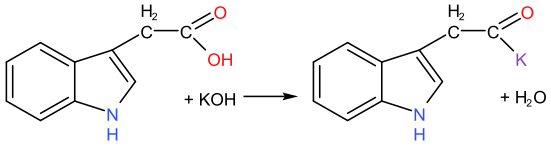


Figure 1. The reaction for obtaining the potassium salt of indole-3-acetic acid

In solution, the selected ligands lose their protons and are converted into IAA^- and AA^- anions. The Zn^{2+} ion possesses vacant coordination orbitals and forms coordination bonds with the IAA^- and AA^- ligands through the oxygen atoms of the carboxylate groups.

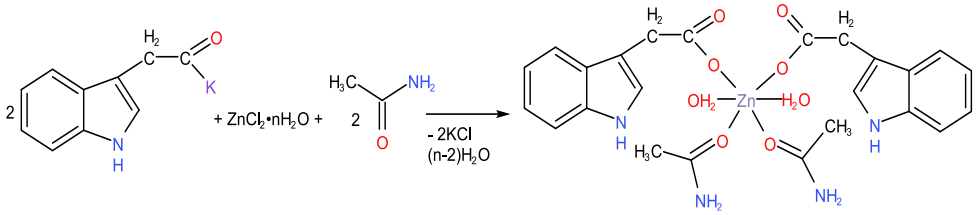


Figure 2. The reaction equation for the formation of the complex compound $[Zn(IAA)_2(AA)_2] \cdot 2H_2O$

As a result, a coordination compound with six coordination and octahedral geometry is formed. During crystallization, the resulting complex incorporates two water molecules, which are considered water of crystallization: $[Zn(IAA)_2(AA)_2] \cdot 2H_2O$.

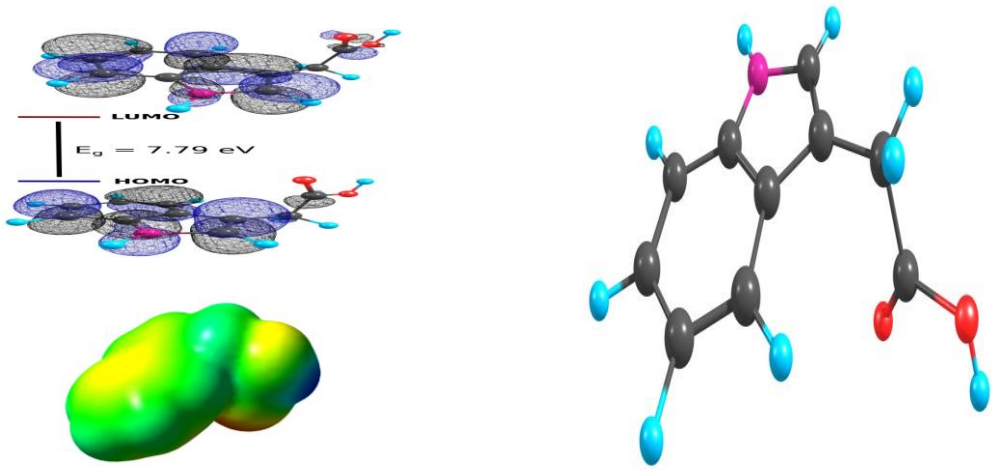
ANALYSIS AND RESULTS. In this study, the electronic structure, geometric parameters, and stability of the synthesized complex $[Zn(IAA)_2(AA)_2] \cdot 2H_2O$ were investigated using quantum chemical calculations. All computations were carried out using the Gaussian program package. The geometry optimization and subsequent analyses were performed within the framework of Density Functional Theory (DFT) employing the range-separated hybrid functional CAM-B3LYP, which is known for its improved description of long-range electron interactions and charge-transfer systems. The initial molecular structure of the complex was constructed based on experimental coordination assumptions, where Zn(II) is coordinated by two indole-3-acetate (IAA^-) and two acetate (AA^-) ligands through oxygen donor atoms. Full geometry optimization was performed without any symmetry constraints, and the nature of the stationary points was confirmed by vibrational frequency analysis, ensuring the absence of imaginary frequencies.

The optimized structure reveals that the Zn(II) center adopts a distorted octahedral coordination environment, where the ligand molecules form stable coordination bonds via carboxylate oxygen atoms. The presence of crystallization water molecules plays an important role in stabilizing the supramolecular structure through hydrogen bonding interactions. Furthermore, frontier molecular orbital (FMO) analysis was carried out to evaluate the electronic properties of the complex. The energies and spatial distributions of HOMO and LUMO orbitals provide insight into the chemical reactivity, kinetic stability, and possible charge-transfer pathways within the complex. The HOMO–LUMO energy gap indicates the relative stability of the system and its potential reactivity. Additionally, charge distribution analysis and electron density mapping were used to better understand the coordination behavior and electron delocalization within the complex system. These results provide a theoretical basis for interpreting the stability and physicochemical properties of the synthesized zinc complex.

Quantum chemical study of ligands and transition metal complex. All quantum chemical calculations were carried out using the Gaussian 16 software package [16]. The molecular geometry was fully optimized in the gas phase without symmetry constraints using the range-separated hybrid functional CAM-B3LYP [17], which incorporates the Coulomb-attenuating method to improve the description of long-range exchange interactions. The LANL2DZ basis set [18] was employed throughout: it applies the Los Alamos National Laboratory double-zeta ECP basis for zinc, treating the inner core electrons through relativistic effective core potentials, while the ligand atoms (C, N, O, H) are described with the standard Dunning/Huzinaga full double-zeta basis. Frequency calculations were performed on the optimized structure to confirm that the geometry corresponds to a true energy minimum on the potential energy surface (absence of imaginary frequencies). Natural bond orbital (NBO) analysis was performed using the NBO 3.1 program interfaced with Gaussian-16 [19] to obtain natural atomic charges, orbital hybridizations, and donor-acceptor interactions via second-

order perturbation theory. Frontier molecular orbitals (HOMO, LUMO) and their energy eigenvalues were extracted from the converged DFT wavefunction. The electrostatic potential was computed on the 0.001 a.u. electron density isosurface and mapped with a color scale ranging from electron-rich (red) to electron-poor (blue) regions.

Electronic structure analysis of ligands.



Electronic structure analysis of Zn(II) complex. Zinc(II) coordination complexes occupy a prominent position in bioinorganic chemistry, materials science, and medicinal chemistry owing to the unique electronic properties of the d^{10} metal center, which confers high thermodynamic stability, Lewis acidity, and favorable luminescence behavior [20]. Unlike transition metals with partially filled d-orbitals, Zn(II) exhibits no d–d transitions, directing all photophysical activity toward ligand-based or ligand-to-metal charge-transfer (LMCT) processes [21].

Indole and its derivatives are biologically privileged scaffolds that appear as constituents of the essential amino acid tryptophan and a broad spectrum of natural products and pharmaceuticals [22]. Their aromatic nitrogen and electron-rich π-system make them excellent candidates for chelation of transition metals, offering both σ-donor N-coordination and π-stacking stabilization [23]. The incorporation of carboxylate and amide functionalities alongside the indole moiety creates multidentate ligand platforms capable of saturating the coordination sphere of Zn(II) while imparting solubility and hydrogen-bonding capacity relevant to aqueous biological environments.

Density functional theory (DFT) has become the standard computational methodology for characterizing the structure, bonding, and reactivity of metal complexes [24]. The range-separated CAM-B3LYP functional is particularly well-suited to zinc coordination compounds, accurately describing charge-transfer excitations and long-range electron correlation effects that are poorly treated by conventional hybrid functionals [25]. The LANL2DZ effective core potential (ECP) basis set provides a computationally efficient treatment of the zinc core electrons while maintaining accuracy for valence-shell properties [26].

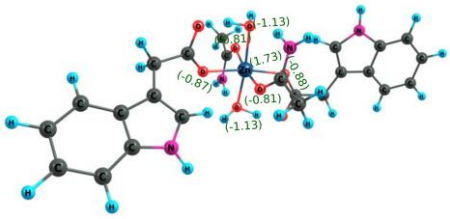


Figure 3. Optimized geometry of the Zn(II) complex at the CAM-B3LYP/LANL2DZ level with NBO partial charges (in parentheses, green text) shown for key donor atoms. Color code: Zn (dark blue), O (red), N (magenta), C (dark gray), H (cyan).

The optimized structure (Figure 3) reveals that the Zn(II) center is hexacoordinate with a strictly oxygen-donor O_6 coordination sphere, adopting a distorted octahedral geometry. The six donor oxygens originate from three chemically distinct sources: two carboxylate oxygens from *indole-2-carboxylic acid* (Zn–O: 2.05 and 2.07 Å), two acetamide carbonyl oxygens from the acetamide-indole ligand (Zn–O: 2.12 and 2.13 Å), and two terminal aqua oxygens (Zn–O: 2.15 and 2.13 Å).

Table 1. Zn–O Bond lengths and NBO charges

Donor Type	Bond 1 (Å)	Bond 2 (Å)	NBO Charge 1 (e)	NBO Charge 2 (e)
Carboxylate O (indole-2-carboxylic acid)	2.05	2.07	−0.87	−0.88
Acetamide O	2.12	2.13	−0.81	−0.81
Terminal O (aqua)	2.15	2.13	−1.13	−1.13
Zn center (NBO)	—	—	+1.73	*(formal: +2.0)*

The NBO charge on zinc (+1.73 e) is reduced by 0.27 e relative to the formal +2 oxidation state, reflecting net ligand-to-metal charge transfer distributed across all six Zn–O bonds. This reduction confirms that the Zn–O bonds are

predominantly ionic with a meaningful covalent component, consistent with Zn(II) acting as a borderline hard Lewis acid with a strong preference for oxygen donors over nitrogen. The carboxylate oxygens of indole-2-carboxylic acid form the shortest bonds in the complex (2.05 and 2.07 Å) and carry moderate negative charges (−0.87 and −0.88 e), identifying them as the strongest σ-donors in the coordination sphere. Their moderate charge magnitudes, rather than extreme values, reflect a balance between inherent oxygen electronegativity, partial charge transfer to Zn, and delocalization across the O–C–O resonance system of the carboxylate. The near-identical values for both oxygens (Δq = 0.01 e, Δd = 0.02 Å) confirm near-symmetric bidentate chelation of indole-2-carboxylic acid. The acetamide carbonyl oxygens exhibit intermediate bond lengths (2.12 and 2.13 Å) and the lowest negative charges among the three oxygen types (−0.81 e each). This is a direct consequence of amide resonance: the nitrogen lone pair adjacent to the C=O group donates electron density into the π*(C=O) orbital ($n_n \rightarrow \pi^*$ interaction), reducing the electron density available on the carbonyl oxygen for metal donation. Both acetamide oxygens are fully equivalent, confirming symmetric coordination geometry. The terminal aqua oxygens present an apparently paradoxical combination of the highest negative charge (−1.13 e) yet the longest Zn–O bonds (2.13–2.15 Å). This is resolved by recognizing that water oxygen retains high negative charge because of the polarization of its two O–H bonds (each H bears ~+0.5 e in NBO), not because of strong donation to zinc.

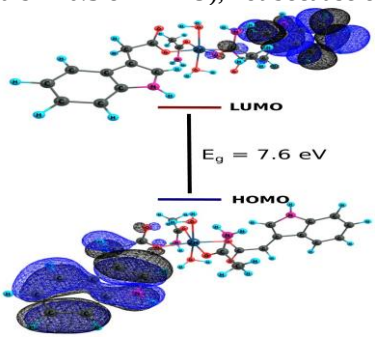


Figure 4. HOMO (bottom) and LUMO (top) of the Zn(II) complex (CAM-B3LYP/LANL2DZ, isovalue = 0.02 a.u.). Blue: positive phase; black mesh: negative phase. E^p = 7.6 eV. Both orbitals are exclusively ligand-centered.

Water is in fact the weakest donor of the three groups, forming the longest and most labile Zn–O bonds. These aqua ligands are therefore the primary sites for ligand exchange in solution and represent the most accessible substitution positions for incoming biological or pharmacological ligands.

The frontier molecular orbitals and HOMO-LUMO gap (E^p = 7.6 eV) are shown in Figure 4. This exceptionally large gap is a direct consequence of the d^{10} configuration of Zn(II): the completely filled d-shell lies well below the HOMO in energy and contributes negligibly to either frontier orbital. All electronic activity is therefore confined to the ligand π-systems. The HOMO is a π-type bonding orbital delocalized across the indole-2-carboxylic acid fragment (left), with alternating lobes above and below the aromatic plane extending over the fused benzene-pyrrole bicyclic system. The indole N–H nitrogen lone pair contributes to the HOMO through conjugation into the aromatic π-system. The LUMO, conversely, is a π*-antibonding orbital localized on the acetamide-indole fragment (right), with the acetamide C=O π* in conjugation with the indole ring. The spatial separation of HOMO and LUMO across the two ligand fragments defines the electronic excitation as a ligand-to-ligand charge transfer (LLCT) process, in which electron density migrates from the indole-2-carboxylic acid side to the acetamide-indole side upon photon absorption, with the Zn center acting as a structural bridge rather than an electronic mediator. The 7.6 eV gap corresponds to a chemical hardness of η = 3.8 eV, classifying this complex as an extremely hard, kinetically stable species.

Electrostatic Potential Surface Analysis is shown in Figure 5.

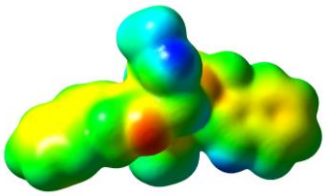


Figure 5. ESP surface of the Zn(II) complex mapped on the 0.001 a.u. electron density isosurface (CAM-B3LYP/LANL2DZ). Red: most electron-rich (negative potential); Blue: most electron-poor (positive potential); Green: near-neutral. Left: indole-2-carboxylic acid fragment; Right: acetamide-indole fragment; Center: O_6 Zn(II) coordination core.

The ESP surface encodes the three-dimensional charge distribution and directly reflects the NBO analysis. The red/orange region concentrated at the central Zn–O coordination core identifies the overlapping lone pairs of the six oxygen donors as the most nucleophilic surface of the molecule, with maximum electron accumulation around the carboxylate and acetamide oxygen atoms consistent with NBO charges of −0.81 to −1.13 e. This zone constitutes the primary hydrogen-bond acceptor and Lewis base surface, reactive toward electrophilic species, metal cations, and proton donors in the surrounding environment. The blue regions at the N–H protons of both indole moieties mark the most electron-deficient sites on the molecular surface. These hydrogen atoms carry positive partial charges due to N–H bond polarization and are strong hydrogen-bond donors, well positioned to interact with Lewis base residues in protein binding

pockets, phosphate groups of DNA/RNA, or carboxylate residues of enzyme active sites. Their moderate acidity also suggests the possibility of deprotonation under basic conditions to form anionic indolate-Zn complexes.

The green coloring across both aromatic ring faces reflects near-neutral π-electron density, consistent with mildly nucleophilic aromatic surfaces capable of π-stacking with nucleobases, cation-π interactions with protonated lysine/arginine residues, and CH-π contacts. A subtle asymmetry is visible: the indole-2-carboxylic acid ring (left) appears slightly greener (more electron-rich) than the acetamide-indole ring (right), consistent with the electron-withdrawing acetamide group reducing π-density on the right fragment—a pattern that also correlates with the LUMO being localized on the right-side ring. The yellow periphery of both ring systems and the aliphatic C–H framework reflects mild positive ESP arising from C–H bond polarization, indicating potential for weak C–H···O hydrogen bonding and van der Waals interactions relevant to crystal packing and biomolecular recognition.

CONCLUSION. The present study reports a quantum chemical investigation of the zinc(II) complex $[Zn(IAA)_2(AA)_2]\cdot 2H_2O$ using Density Functional Theory calculations performed with the Gaussian program package. Geometry optimizations and electronic structure analyses were carried out at the CAM-B3LYP/LANL2DZ level of theory, confirming a stable optimized structure without imaginary frequencies. The results show that Zn(II) forms a six-coordinate distorted octahedral geometry with oxygen donor atoms. NBO analysis indicates predominantly ionic Zn–O interactions with partial covalent character due to ligand-to-metal charge transfer. Frontier molecular orbital analysis reveals a ligand-centered electronic structure with a large HOMO–LUMO gap (7.6 eV), indicating high kinetic stability and low reactivity. Electrostatic potential mapping further identifies oxygen atoms as the main reactive sites in the complex. Overall, the obtained theoretical results provide a consistent description of the structural stability and electronic properties of the synthesized zinc(II) complex, supporting its potential relevance in coordination and bioinorganic chemistry.

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Annotatsiya. Maqolada rux(II) ioni bilan indol-3-sirka kislotasi (geteroauksin) va atsetamid asosidagi yangi aralash ligandli koordinatsion birikmaning sintezi tavsiflangan. Olingan kompleks birikmaning tarkibi va tuzilishi element tahlili hamda IQ-spektroskopiya usullari yordamida tadqiq etildi. IQ-spektrlar tahlili ligandlarning metal ioniga koordinatsiyalanish usullarini aniqlash imkonini berdi. Tadqiqotning ikkinchi qismida kompleksning elektron tuzilishi va termodinamik xarakteristikalari kvant-kimyoviy hisoblashlar (DFT usuli) yordamida tahlil qilindi. Natijalar nazariy va tajribaviy ma'lumotlar o‘rtasida yuqori korrelyatsiya mavjudligini ko‘rsatdi, bu esa sintez qilingan kompleksning potentsial biologik faolligi uchun asos bo‘lib xizmat qiladi.

Kalit so‘zlar: rux(II), indol-3-sirka kislotasi, atsetamid, koordinatsion birikma, sintez, IQ-spektroskopiya.

Аннотация. В статье описан синтез нового смешаннолигандного координационного соединения иона цинка(II) с индол-3-уксусной кислотой (гетероауксином) и ацетамидом. Состав и структура полученного комплексного соединения были исследованы с помощью элементного анализа и ИК-спектроскопии. Анализ ИК-спектров позволил определить способы координации лигандов к иону металла. Во второй части исследования с помощью квантово-химических расчетов (метод DFT) были проанализированы электронное строение и термодинамические характеристики комплекса. Результаты демонстрируют высокую корреляцию между теоретическими и экспериментальными данными, что дает основание для прогнозирования потенциальной биологической активности синтезированного комплекса.

Ключевые слова: цинк(II), индол-3-уксусная кислота, ацетамид, координационное соединение, синтез, ИК-спектроскопия.

Abstract. The article describes the synthesis of a new mixed-ligand coordination compound of zinc(II) ion with indole-3-acetic acid (heteroauxin) and acetamide. The composition and structure of the obtained complex compound were investigated using elemental analysis and IR spectroscopy. Analysis of the IR spectra allowed determining the coordination modes of the ligands to the metal ion. In the second part of the study, the electronic structure and thermodynamic characteristics of the complex were analyzed using quantum-chemical calculations (DFT method). The results show a high correlation between theoretical and experimental data, providing a basis for the potential biological activity of the synthesized complex.

Keywords: zinc(II), indole-3-acetic acid, acetamide, coordination compound, synthesis, IR spectroscopy.