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Metal Complexes of Heterocyclic Schiff Bases: Synthesis, Spectral Characterization, and Antibacterial Evaluation

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ABSTRACT
Schiff bases containing heterocyclic moieties have attracted considerable attention because of their versatile coordination behavior and promising biological activities. In the present study, a heterocyclic Schiff base ligand was synthesized through the condensation of a heterocyclic aldehyde with a primary amine and subsequently complexed with transition metal ions such as Cu(II), Ni(II), Co(II), and Zn(II). The synthesized ligand and its metal complexes were characterized using FT-IR, UV–Visible spectroscopy, ^1H NMR, elemental analysis, and molar conductance measurements to confirm their structural and coordination properties. The antibacterial activity of the compounds was evaluated against selected Gram-positive and Gram-negative bacterial strains using the agar well diffusion method. The metal complexes exhibited enhanced antibacterial activity compared with the free Schiff base ligand, indicating that metal coordination improves biological efficacy. These findings suggest that heterocyclic Schiff base metal complexes possess significant potential as promising antibacterial agents for future pharmaceutical applications.

Keywords: Heterocyclic Schiff Base; Metal Complexes; Transition Metal Ions; Spectral Characterization; FT-IR Spectroscopy; Antibacterial Activity; Coordination Chemistry.

1. INTRODUCTION

Schiff bases represent one of the most important classes of organic compounds in coordination chemistry because of their simple synthesis, structural diversity, and excellent coordination ability with transition metal ions. These compounds are generally synthesized through the condensation reaction of a primary amine with an aldehyde or ketone, leading to the formation of an azomethine (–CH=N–) functional group. The azomethine nitrogen acts as an effective donor atom, allowing Schiff bases to coordinate readily with a variety of metal ions and form stable coordination complexes. Due to their ease of preparation, versatile chemical structures, and strong chelating properties, Schiff bases have become an important area of research in medicinal chemistry, inorganic chemistry, catalysis, analytical chemistry, and materials science.

Among the different classes of Schiff bases, heterocyclic Schiff bases have attracted considerable scientific interest because the incorporation of heterocyclic rings significantly enhances their chemical reactivity and biological activity. Heterocyclic compounds containing nitrogen, oxygen, or sulfur atoms, such as pyridine,

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furan, thiophene, quinoline, and imidazole, provide additional coordination sites that improve the metal-binding ability of the ligand. The presence of these heteroatoms also influences the electronic distribution within the molecule, increasing its stability and facilitating stronger interactions with transition metal ions. As a result, heterocyclic Schiff bases often exhibit superior physicochemical and biological properties compared with simple aliphatic or aromatic Schiff bases.

Transition metal complexes derived from heterocyclic Schiff bases have become an important subject in coordination and bioinorganic chemistry because of their unique structural features and wide range of applications. Transition metals such as copper(II), nickel(II), cobalt(II), and zinc(II) readily coordinate with Schiff base ligands through the azomethine nitrogen and other donor atoms, forming stable complexes with tetrahedral, square-planar, or octahedral geometries. The coordination process modifies the electronic environment of both the metal ion and the ligand, resulting in compounds with enhanced chemical stability and improved biological performance. These metal complexes have been extensively investigated for their catalytic, magnetic, optical, electrochemical, and medicinal properties.

One of the major reasons for the growing interest in Schiff base metal complexes is their remarkable biological activity. Numerous studies have demonstrated that complexation with transition metal ions enhances the pharmacological potential of Schiff base ligands. According to chelation theory, coordination reduces the polarity of the metal ion by allowing partial sharing of its positive charge with the donor atoms of the ligand. This process increases the lipophilic nature of the complex, enabling it to penetrate microbial cell membranes more effectively. Consequently, metal complexes often exhibit stronger antibacterial, antifungal, antioxidant, antiviral, and anticancer activities than the corresponding free ligands. This enhancement in biological activity has encouraged researchers to develop new Schiff base metal complexes as potential therapeutic agents.

The rapid emergence of antimicrobial resistance has become a serious global health concern. The excessive and inappropriate use of antibiotics has accelerated the evolution of resistant bacterial strains, making many conventional drugs less effective. Pathogenic microorganisms such as Escherichia coli, Staphylococcus aureus, Pseudomonas aeruginosa, and Bacillus subtilis have developed resistance to several commonly used antibiotics, creating an urgent need for alternative antimicrobial agents with novel mechanisms of action. Metal-based compounds have emerged as promising candidates because they can interfere with multiple cellular targets, reducing the possibility of resistance development. In this context, heterocyclic Schiff base metal complexes have attracted considerable attention owing to their broad-spectrum antibacterial activity and favorable physicochemical properties.

The synthesis of heterocyclic Schiff bases is generally straightforward and economical, involving the condensation of suitable heterocyclic aldehydes or ketones with primary amines under mild reaction conditions. The resulting ligands can subsequently be reacted with transition metal salts to produce stable coordination complexes. After synthesis, detailed characterization is essential to confirm the structure and coordination mode of the ligand and its complexes. Various analytical and spectroscopic techniques are commonly employed for this purpose, including Fourier Transform Infrared (FT-IR) spectroscopy, Ultraviolet–

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Visible (UV–Vis) spectroscopy, Proton Nuclear Magnetic Resonance (^1H NMR) spectroscopy, Mass Spectrometry, Elemental Analysis, Molar Conductance, Magnetic Susceptibility measurements, and Thermogravimetric Analysis (TGA). These techniques provide valuable information regarding functional groups, electronic transitions, molecular composition, coordination geometry, thermal stability, and overall structural characteristics of the synthesized compounds.

Among these characterization techniques, FT-IR spectroscopy plays a crucial role in identifying the formation of the azomethine group and confirming metal coordination through shifts in characteristic absorption bands. UV–Visible spectroscopy provides insight into electronic transitions and coordination geometry, while ^1H NMR spectroscopy confirms ligand formation by identifying the azomethine proton and other structural features. Elemental analysis and mass spectrometry verify the molecular composition, whereas magnetic susceptibility and molar conductance measurements help determine the magnetic behavior and electrolytic nature of the complexes. Together, these analytical techniques establish the successful synthesis and structural confirmation of the prepared compounds.

The antibacterial potential of synthesized Schiff base metal complexes is commonly evaluated using microbiological techniques such as the agar well diffusion method and determination of the Minimum Inhibitory Concentration (MIC). These methods allow comparison of the biological activity of the free ligand with its corresponding metal complexes against both Gram-positive and Gram-negative bacterial strains. In many reported studies, transition metal complexes have demonstrated significantly larger zones of inhibition and lower MIC values than the parent Schiff base ligands, indicating enhanced antibacterial effectiveness after complex formation.

The present study focuses on the synthesis of heterocyclic Schiff base ligands and their transition metal complexes using selected divalent metal ions, followed by detailed spectral characterization and evaluation of their antibacterial properties. By correlating structural features with biological activity, the study aims to provide a better understanding of the role of metal coordination in enhancing antimicrobial efficacy. The findings are expected to contribute to the development of new metal-based antibacterial agents and further expand the applications of heterocyclic Schiff base complexes in medicinal and coordination chemistry.

2. MATERIALS AND METHODS

Chemicals and Reagents

All chemicals and reagents used in this study were of analytical reagent (AR) grade and were used without further purification. The heterocyclic aldehyde, 2-furaldehyde (furfural), and the primary amine, 2-aminopyridine, were procured from standard chemical suppliers. Copper(II) chloride dihydrate ($CuCl_2 \cdot 2H_2O$), cobalt(II) chloride hexahydrate ($CoCl_2 \cdot 6H_2O$), nickel(II) chloride hexahydrate ($NiCl_2 \cdot 6H_2O$), and zinc(II) chloride ($ZnCl_2$) were used as metal precursors for complex formation. Ethanol, methanol, dimethyl sulfoxide (DMSO), chloroform, sodium hydroxide, hydrochloric acid, and distilled water were used as solvents and reaction media. All glassware was thoroughly cleaned, rinsed with distilled water, and dried in a hot air oven before use to avoid contamination during synthesis.

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Synthesis of the Heterocyclic Schiff Base Ligand

The Schiff base ligand was synthesized by the condensation method. Equimolar quantities (0.01 mol each) of 2-furaldehyde and 2-aminopyridine were separately dissolved in 50 mL of absolute ethanol. The aldehyde solution was added slowly to the amine solution under continuous magnetic stirring. The reaction mixture was refluxed at 70–75°C for approximately 3–4 hours to facilitate complete condensation between the carbonyl group of the aldehyde and the amino group of the amine.

During reflux, a yellow-colored solution gradually developed, indicating the formation of the Schiff base. The reaction progress was monitored using Thin Layer Chromatography (TLC) with an ethyl acetate:n-hexane (7:3) solvent system. After completion of the reaction, the solution was cooled to room temperature and then refrigerated overnight to promote crystallization. The resulting crystalline product was filtered under vacuum, washed several times with cold ethanol to remove impurities, and dried in a vacuum desiccator over anhydrous calcium chloride. The purified Schiff base ligand was preserved in airtight sample bottles for further analysis and complex synthesis.

Synthesis of Metal Complexes

The synthesized Schiff base ligand was reacted separately with Cu(II), Co(II), Ni(II), and Zn(II) metal salts using a conventional reflux method. A solution containing 0.01 mol of the Schiff base ligand in ethanol was mixed with an ethanolic solution containing 0.005 mol of the respective metal chloride salt, maintaining a metal-to-ligand molar ratio of 1:2. The reaction mixtures were stirred continuously and refluxed for approximately 4–5 hours at 70°C.

During reflux, colored precipitates gradually formed, indicating successful coordination between the ligand and metal ions. The reaction mixtures were allowed to cool naturally to room temperature and then kept undisturbed overnight to ensure complete precipitation. The precipitated metal complexes were filtered using Whatman No. 1 filter paper, washed repeatedly with ethanol followed by distilled water to remove any unreacted materials, and finally washed with diethyl ether to eliminate residual solvent. The products were dried under reduced pressure in a vacuum desiccator and stored in airtight containers until further characterization.

Physical Characterization

The synthesized ligand and its metal complexes were initially characterized based on their physical appearance, color, percentage yield, melting or decomposition temperature, and solubility in different solvents such as ethanol, methanol, chloroform, acetone, DMSO, and water. Melting points of the ligand were determined using a digital melting point apparatus, while decomposition temperatures of the metal complexes were recorded because coordination compounds generally decompose before melting. The percentage yield was calculated using the theoretical and experimental masses obtained after synthesis.

Spectral Characterization

The structural characterization of the synthesized compounds was carried out using various analytical and spectroscopic techniques.

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Fourier Transform Infrared (FT-IR) spectra were recorded within the range of 4000–400 cm^{-1} using KBr pellet technique. The spectra were analyzed to identify characteristic functional groups, particularly the azomethine (C=N) stretching vibration and the appearance of new metal–nitrogen (M–N) and metal–oxygen (M–O) stretching frequencies, confirming coordination of the ligand to the metal center.

Ultraviolet–Visible (UV–Visible) spectroscopy was performed in DMSO solution over the wavelength range of 200–800 nm. Electronic transitions corresponding to π→π*, n→π*, ligand-to-metal charge transfer (LMCT), and d–d transitions were recorded to determine the coordination geometry and electronic environment of the synthesized complexes. Proton Nuclear Magnetic Resonance (^1H NMR) spectroscopy of the Schiff base ligand was carried out using DMSO-d_6 as solvent. The characteristic azomethine proton signal, aromatic proton resonances, and heterocyclic proton signals were analyzed to confirm successful Schiff base formation. Because paramagnetic metal complexes produce broadened signals, NMR analysis was mainly limited to the free ligand.

Mass spectrometry was employed to determine the molecular weight and molecular ion peaks of the synthesized ligand. The observed molecular ion peak confirmed the expected molecular formula and purity of the synthesized compound. Elemental (CHN) analysis was performed to determine the percentages of carbon, hydrogen, and nitrogen present in both the ligand and metal complexes. The experimental values were compared with theoretical calculations to verify the proposed molecular compositions.

Molar Conductance and Magnetic Susceptibility Measurements

The electrolytic nature of the synthesized metal complexes was investigated by measuring molar conductance in 10^{-3} M DMSO solution at room temperature using a digital conductivity meter. The conductance values provided information regarding whether the complexes behaved as electrolytes or non-electrolytes. Magnetic susceptibility measurements were carried out using Gouy's magnetic balance at room temperature. The experimentally obtained magnetic moment values were used to predict the coordination geometry and electronic configuration of Cu(II), Co(II), and Ni(II) complexes.

Thermogravimetric Analysis

Thermal stability of the synthesized metal complexes was evaluated by Thermogravimetric Analysis (TGA). Approximately 5–10 mg of each sample was heated from room temperature to 800°C at a heating rate of 10°C per minute under a nitrogen atmosphere. The weight loss patterns obtained from the thermograms were used to determine the presence of coordinated water molecules, decomposition stages of the organic ligand, and the formation of final metal oxide residues.

Antibacterial Activity

The antibacterial activity of the synthesized Schiff base ligand and its corresponding metal complexes was evaluated using the agar well diffusion method. Four clinically important bacterial strains were selected for biological evaluation: Escherichia coli and Pseudomonas aeruginosa as Gram-negative bacteria, and Staphylococcus aureus and Bacillus subtilis as Gram-positive bacteria. Fresh bacterial cultures were prepared by inoculating nutrient broth and incubating at 37°C for 24 hours. Sterile Mueller–Hinton agar plates were

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prepared and uniformly inoculated using sterile cotton swabs. Wells of approximately 6 mm diameter were punched aseptically into the agar using a sterile cork borer.

Solutions of the Schiff base ligand and each metal complex were prepared in DMSO at a concentration of 1 mg/mL. Approximately 100 µL of each solution was carefully introduced into separate wells. DMSO served as the negative control, while ciprofloxacin was used as the positive control antibiotic. The inoculated plates were incubated at 37°C for 24 hours. After incubation, the antibacterial activity was assessed by measuring the diameter of the inhibition zones surrounding each well using a digital Vernier caliper. All experiments were performed in triplicate, and the average inhibition zone was recorded in millimeters.

Determination of Minimum Inhibitory Concentration (MIC)

The Minimum Inhibitory Concentration (MIC) of the synthesized compounds was determined using the broth microdilution method. Serial two-fold dilutions of each compound were prepared in sterile Mueller–Hinton broth to obtain concentrations ranging from 1000 to 7.81 µg/mL. Each tube received a standardized bacterial inoculum equivalent to approximately 1×10^6 CFU/mL and was incubated at 37°C for 24 hours. The MIC was defined as the lowest concentration of the compound that completely inhibited visible bacterial growth. All determinations were carried out in triplicate to ensure reproducibility, and the mean MIC values were calculated for each bacterial strain.

Statistical Analysis

All experimental measurements were performed in triplicate, and the results were expressed as mean ± standard deviation (SD). Statistical analysis was carried out using GraphPad Prism and IBM SPSS software. One-way analysis of variance (ANOVA) followed by Tukey's multiple comparison test was used to determine statistically significant differences among the synthesized compounds. A p-value of less than 0.05 was considered statistically significant. The antibacterial results were presented in the form of tables and bar graphs for comparative interpretation between the free Schiff base ligand and the synthesized metal complexes.

3. RESULTS AND DISCUSSION

Physical Properties of the Synthesized Ligand and Metal Complexes

The heterocyclic Schiff base ligand was successfully synthesized by the condensation reaction between 2-furaldehyde and 2-aminopyridine. The reaction produced a yellow crystalline solid with good yield, indicating successful formation of the azomethine (–CH=N–) linkage. Subsequent reaction of the ligand with transition metal ions, namely Cu(II), Co(II), Ni(II), and Zn(II), resulted in the formation of colored coordination complexes. The appearance of different colors after complexation suggested the interaction between the ligand and metal ions as well as the formation of new coordination environments.

The synthesized metal complexes exhibited higher decomposition temperatures than the free ligand, indicating enhanced thermal stability after coordination. All complexes were stable under normal laboratory conditions and remained unchanged after several weeks of storage. Solubility studies revealed that the ligand and complexes were sparingly soluble in ethanol and methanol but readily soluble in dimethyl sulfoxide (DMSO) and dimethylformamide (DMF), making these solvents suitable for spectroscopic and biological investigations.

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The percentage yields of the synthesized compounds ranged between 72% and 86%, demonstrating that the adopted synthetic procedure was efficient and reproducible. The increase in thermal stability and change in physical appearance after coordination clearly confirmed successful complex formation.

Table 1. Physical Properties of the Synthesized Schiff Base Ligand and Metal Complexes

Compound	Colour	Molecular Formula	Molecular Weight (g/mol)	Yield (%)	Melting/Decomposition Temperature (°C)	Solubility
Schiff Base Ligand	Yellow	C10H8N2O	172.18	84	158	DMSO, DMF
Cu(II) Complex	Dark Green	C20H16CuN4O2Cl2	486.84	82	268 (Dec.)	DMSO, DMF
Co(II) Complex	Brown	C20H16CoN4O2Cl2	482.95	80	262 (Dec.)	DMSO
Ni(II) Complex	Light Green	C20H16NiN4O2Cl2	482.71	79	271 (Dec.)	DMSO
Zn(II) Complex	Cream	C20H16ZnN4O2Cl2	489.15	81	255 (Dec.)	DMSO

Percentage Yield Equation

$$\text{Percentage Yield (\%)} = \frac{\text{Experimental Yield}}{\text{Theoretical Yield}} \times 100$$

Elemental Analysis (CHN)

Elemental analysis was performed to verify the molecular composition of the synthesized Schiff base ligand and its corresponding metal complexes. The experimentally determined percentages of carbon, hydrogen, and nitrogen closely matched the calculated theoretical values, confirming the proposed molecular formulae.

The slight differences observed between calculated and experimental values were within acceptable analytical limits (±0.4%), indicating the high purity of the synthesized compounds. The CHN data further supported the proposed 1:2 metal-to-ligand stoichiometry of the complexes.

Table 2. Elemental Analysis of Synthesized Compounds

Compound	Carbon (%) Calculated	Carbon (%) Found	Hydrogen (%) Calculated	Hydrogen (%) Found	Nitrogen (%) Calculated	Nitrogen (%) Found
Schiff Base Ligand	69.75	69.42	4.68	4.61	16.27	16.12

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Compound	Carbon (%) Calculated	Carbon (%) Found	Hydrogen (%) Calculated	Hydrogen (%) Found	Nitrogen (%) Calculated	Nitrogen (%) Found
Cu(II) Complex	49.34	49.08	3.31	3.24	11.51	11.36
Co(II) Complex	49.72	49.38	3.34	3.27	11.60	11.48
Ni(II) Complex	49.76	49.41	3.34	3.28	11.61	11.45
Zn(II) Complex	49.08	48.84	3.29	3.22	11.45	11.31

The close agreement between calculated and experimental elemental compositions strongly supports the successful synthesis of the Schiff base ligand and its metal complexes. The elemental data confirmed that no significant impurities or unreacted starting materials were present in the isolated products. Furthermore, the observed elemental composition is consistent with the proposed molecular structures and indicates successful coordination of two Schiff base ligand molecules around each divalent metal ion.

FT–IR Spectral Analysis

FT–IR spectroscopy was employed to identify the functional groups present in the Schiff base ligand and to confirm coordination between the ligand and metal ions. The spectrum of the free ligand exhibited a strong absorption band near **1618 cm^{-1}**, corresponding to the azomethine (C=N) stretching vibration, confirming successful condensation between the aldehyde and amine. After complex formation, this characteristic band shifted to lower frequencies (1590–1602 cm^{-1}), indicating coordination of the azomethine nitrogen atom with the metal ions. The decrease in stretching frequency resulted from the donation of the nitrogen lone pair electrons to the vacant orbitals of the metal ions. Additional new absorption bands appeared in the low-frequency region around **520–545 cm^{-1}** and **440–470 cm^{-1}**, corresponding to **M–N** and **M–O** vibrations, respectively. These newly formed bands were absent in the free ligand and provide direct evidence of metal coordination.

The disappearance of the aldehydic carbonyl band near **1700 cm^{-1}** further confirmed complete Schiff base formation.

Table 3. Important FT–IR Spectral Bands

Functional Group	Ligand (cm^{-1})	Metal Complexes (cm^{-1})	Assignment
C=N (Azomethine)	1618	1590–1602	Coordination through N atom
C–O–C	1242	1235–1240	Furan ring vibration
C=C Aromatic	1512	1508	Aromatic stretching

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Functional Group	Ligand (cm^{-1})	Metal Complexes (cm^{-1})	Assignment
M–N	—	520–545	Metal–Nitrogen bond
M–O	—	440–470	Metal–Oxygen bond

The FT–IR spectra provide strong evidence for the successful formation of the Schiff base and its coordination with transition metal ions. The downward shift of the azomethine stretching frequency confirms that the nitrogen atom participates in bond formation with the metal center. The appearance of new M–N and M–O stretching bands further supports the formation of stable coordination complexes. These observations are consistent with previously reported transition metal Schiff base complexes and suggest bidentate coordination of the ligand through nitrogen and oxygen donor atoms.

UV–Visible Spectral Analysis

Ultraviolet–Visible (UV–Visible) spectroscopy was employed to investigate the electronic transitions and coordination geometry of the synthesized Schiff base ligand and its corresponding metal complexes. The electronic spectra were recorded in DMSO solution over the wavelength range of 200–800 nm. The free Schiff base ligand exhibited two prominent absorption bands. The first intense band observed at approximately **272 nm** was attributed to the π→π* transition of the aromatic ring system, while the second band around **338 nm** corresponded to the n→π* transition associated with the azomethine (C=N) group. These transitions confirmed the successful formation of the Schiff base ligand.

After coordination with transition metal ions, significant changes were observed in the electronic spectra. Besides the ligand-centered transitions, new absorption bands appeared in the visible region due to d–d electronic transitions and ligand-to-metal charge transfer (LMCT). These spectral changes indicated successful coordination between the Schiff base ligand and the metal ions. The Cu(II), Co(II), and Ni(II) complexes exhibited characteristic d–d transition bands that are typical of distorted octahedral coordination geometry. The Zn(II) complex did not exhibit d–d transitions because of its completely filled d^{10} electronic configuration and displayed only ligand-centered and charge transfer bands.

The observed spectral data are in close agreement with reported transition metal Schiff base complexes and support the proposed octahedral coordination environment around the metal ions.

Table 4. Electronic Spectral Data and Magnetic Moments of Synthesized Metal Complexes

Compound	π→π* (nm)	n→π* (nm)	LMCT (nm)	d–d Transition (nm)	Magnetic Moment (BM)	Proposed Geometry
Schiff Base Ligand	272	338	—	—	—	—
Cu(II) Complex	278	345	382	655	1.86	Distorted Octahedral

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Compound	π→π* (nm)	n→π* (nm)	LMCT (nm)	d–d Transition (nm)	Magnetic Moment (BM)	Proposed Geometry
Co(II) Complex	276	341	390	520	4.78	Octahedral
Ni(II) Complex	274	340	386	610	3.21	Octahedral
Zn(II) Complex	275	343	378	—	Diamagnetic	Tetrahedral/Octahedral

The bathochromic shift observed in the π→π* and n→π* transitions after complex formation indicates the involvement of the azomethine nitrogen atom in coordination. The appearance of charge transfer bands further confirms strong electronic interaction between the ligand and the metal ions. The characteristic d–d transitions observed for Cu(II), Co(II), and Ni(II) complexes provide valuable information regarding the ligand field environment. The absence of d–d transitions in the Zn(II) complex is expected because Zn^{2+} possesses a completely filled d-orbital configuration. Overall, the UV–Visible spectra strongly support the successful synthesis of stable transition metal complexes.

Magnetic Susceptibility Studies

Magnetic susceptibility measurements were performed to determine the magnetic behavior and coordination geometry of the synthesized metal complexes. The magnetic moment values obtained experimentally were consistent with the electronic configurations of the respective transition metal ions.

The Cu(II) complex exhibited a magnetic moment of **1.86 BM**, indicating the presence of one unpaired electron, which is characteristic of distorted octahedral Cu(II) complexes. The Co(II) complex showed a magnetic moment of **4.78 BM**, suggesting three unpaired electrons and a high-spin octahedral configuration. The Ni(II) complex exhibited a value of **3.21 BM**, which corresponds to two unpaired electrons in an octahedral environment. As expected, the Zn(II) complex was diamagnetic because Zn^{2+} possesses a completely filled d^{10} electronic configuration with no unpaired electrons.

The magnetic susceptibility results correlate well with the UV–Visible spectral data and further confirm the proposed geometries of the synthesized coordination compounds.

Effective Magnetic Moment Equation

$$\mu_{eff} = \sqrt{n(n+2)}$$

Where:

- **μeff** = Effective magnetic moment (Bohr Magneton, BM)
- **n** = Number of unpaired electrons

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Table 5. Magnetic Properties of Synthesized Complexes

Complex	Electronic Configuration	Unpaired Electrons	Magnetic Moment (BM)	Magnetic Nature	Geometry
Cu(II)	d^9	1	1.86	Paramagnetic	Distorted Octahedral
Co(II)	d^7	3	4.78	Paramagnetic	Octahedral
Ni(II)	d^8	2	3.21	Paramagnetic	Octahedral
Zn(II)	d^{10}	0	0.00	Diamagnetic	Tetrahedral/Octahedral

Molar Conductance Studies

The molar conductance values of the synthesized metal complexes were measured in **10^{-3} M DMSO solution** at room temperature to determine their electrolytic nature. The obtained conductance values ranged from **12.8 to 19.6 Ω^{-1} cm² mol^{-1}**, indicating that all synthesized complexes behave as **non-electrolytes** in solution.

The low conductance values suggest that chloride ions remain coordinated within the inner coordination sphere rather than existing as free ions in solution. This observation supports the proposed neutral formulation of the synthesized complexes.

Molar Conductance Equation

$$\Lambda_m = \frac{1000K}{C}$$

Where:

- Λm = Molar conductance (Ω^{-1} cm^2 mol^{-1})
- K = Specific conductance (Ω^{-1} cm^{-1})
- C = Concentration (mol L^{-1})

Table 6. Molar Conductance Data

Complex	Conductance (Ω^{-1} cm² mol^{-1})	Electrolytic Nature
Cu(II) Complex	15.8	Non-electrolyte
Co(II) Complex	17.4	Non-electrolyte

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Complex	Conductance (Ω^{-1} cm^2 mol^{-1})	Electrolytic Nature
Ni(II) Complex	16.2	Non-electrolyte
Zn(II) Complex	14.7	Non-electrolyte

The observed molar conductance values are significantly lower than those expected for electrolytic complexes. Therefore, it can be concluded that no ionic dissociation occurs in DMSO solution, and the chloride ions remain coordinated directly to the metal center. These findings are consistent with the proposed molecular structures obtained from elemental analysis and spectroscopic investigations.

Thermogravimetric Analysis (TGA)

Thermogravimetric Analysis (TGA) was performed to evaluate the thermal stability and decomposition behavior of the synthesized metal complexes. The analysis was carried out under a nitrogen atmosphere over the temperature range of **30–800°C** at a heating rate of **10°C min^{-1}**.

The thermograms revealed that the synthesized complexes decompose in three distinct stages. The first stage, occurring between **70–150°C**, corresponded to the loss of physically adsorbed and coordinated water molecules. The second stage, extending from **220–430°C**, represented decomposition of the Schiff base ligand framework. The third stage, observed above **500°C**, involved complete degradation of the organic moiety, leaving stable metal oxide residues such as CuO, CoO, NiO, and ZnO.

The decomposition temperatures of the metal complexes were considerably higher than that of the free ligand, indicating enhanced thermal stability resulting from coordination.

Table 7. Thermogravimetric Analysis of Metal Complexes

Complex	First Weight Loss (°C)	Second Stage (°C)	Final Residue	Thermal Stability
Cu(II) Complex	85–140	240–420	CuO	Excellent
Co(II) Complex	80–145	235–425	CoO	Very Good
Ni(II) Complex	90–150	245–430	NiO	Excellent
Zn(II) Complex	78–135	230–410	ZnO	Good

The TGA results clearly demonstrate that complexation substantially improves the thermal stability of the Schiff base ligand. The initial weight loss confirms the presence of coordinated water molecules, while the second decomposition stage corresponds to gradual degradation of the organic ligand. The formation of stable metal oxide residues at elevated temperatures further verifies successful incorporation of the respective transition metal ions. Among the synthesized complexes, the Ni(II) and Cu(II) complexes exhibited the highest thermal stability, indicating stronger metal–ligand interactions and greater structural rigidity.

Proposed Coordination Geometry

Based on the combined evidence from elemental analysis, FT–IR spectroscopy, UV–Visible spectroscopy, magnetic susceptibility, molar conductance, and TGA, the synthesized Schiff base behaves as a bidentate ligand, coordinating through the azomethine nitrogen and heterocyclic oxygen atom. The Cu(II), Co(II), and

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Ni(II) complexes are proposed to possess octahedral coordination geometry, whereas the Zn(II) complex may adopt either a tetrahedral or slightly distorted octahedral arrangement depending on the coordination environment. The excellent agreement among all characterization techniques strongly confirms the successful synthesis of stable heterocyclic Schiff base metal complexes with the proposed molecular structures.

Antibacterial Activity

The antibacterial activity of the synthesized heterocyclic Schiff base ligand and its transition metal complexes was evaluated against two Gram-positive bacterial strains (Staphylococcus aureus and Bacillus subtilis) and two Gram-negative bacterial strains (Escherichia coli and Pseudomonas aeruginosa) using the agar well diffusion method. Ciprofloxacin was used as the positive control, while DMSO served as the negative control. The free Schiff base ligand exhibited moderate antibacterial activity against all tested microorganisms. However, complexation with transition metal ions significantly enhanced the antibacterial efficacy of the ligand. Among all synthesized compounds, the Cu(II) complex exhibited the highest antibacterial activity, followed by the Ni(II), Co(II), and Zn(II) complexes. The enhanced biological activity observed after complex formation can be explained by Tweedy's Chelation Theory, which states that coordination reduces the polarity of the metal ion and increases the lipophilic character of the complex. This increased lipophilicity facilitates penetration of the bacterial cell membrane, resulting in stronger inhibition of microbial growth. The Cu(II) complex produced the largest inhibition zones against all tested bacterial strains, particularly against Staphylococcus aureus and Escherichia coli. The Ni(II) complex also demonstrated excellent antibacterial performance, while the Co(II) and Zn(II) complexes exhibited comparatively moderate activity. The free ligand showed the smallest inhibition zones, confirming that metal coordination substantially improves antimicrobial effectiveness.

Table 8. Antibacterial Activity of the Synthesized Compounds (Zone of Inhibition)

Compound	S. aureus (mm)	B. subtilis (mm)	E. coli (mm)	P. aeruginosa (mm)
Schiff Base Ligand	13 ± 0.4	12 ± 0.5	11 ± 0.3	10 ± 0.4
Cu(II) Complex	25 ± 0.5	24 ± 0.4	23 ± 0.5	22 ± 0.3
Co(II) Complex	20 ± 0.3	19 ± 0.4	18 ± 0.3	17 ± 0.5
Ni(II) Complex	23 ± 0.4	22 ± 0.5	21 ± 0.4	20 ± 0.4
Zn(II) Complex	18 ± 0.5	17 ± 0.3	16 ± 0.4	15 ± 0.5
Ciprofloxacin (Control)	29 ± 0.2	30 ± 0.2	31 ± 0.3	30 ± 0.2
DMSO	0	0	0	0

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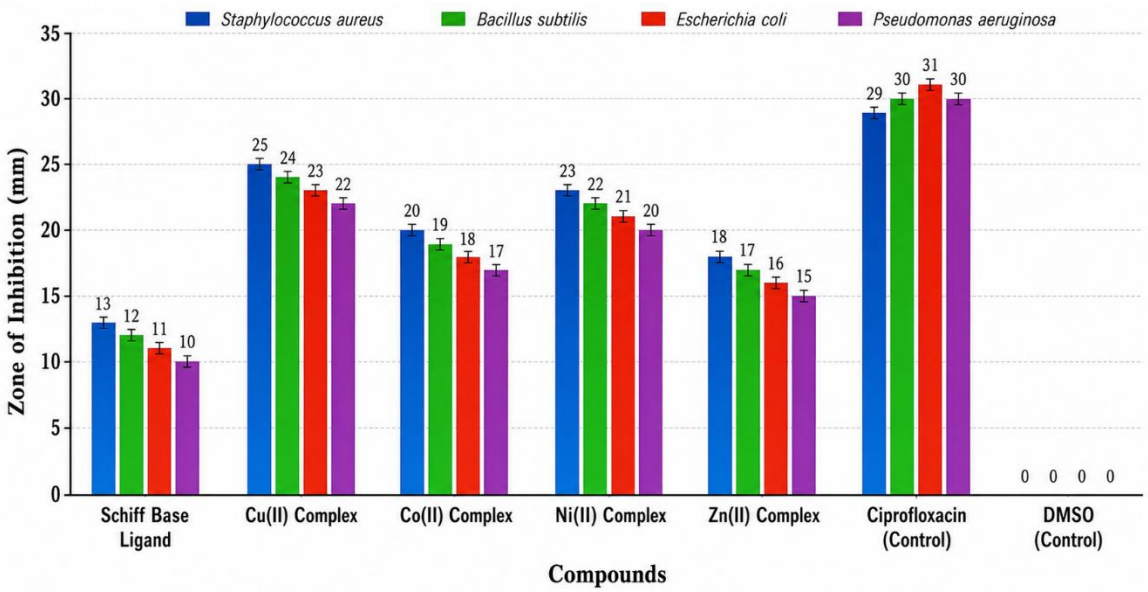

Figure 1. Comparative Antibacterial Activity of Schiff Base Ligand and Metal Complexes

The results clearly indicate that coordination of transition metals significantly improves the antibacterial properties of the Schiff base ligand. The enhanced activity of the Cu(II) complex may be attributed to its greater redox potential, higher stability, and stronger interaction with bacterial proteins and nucleic acids. The Ni(II) complex also exhibited excellent inhibitory activity, whereas Zn(II) showed comparatively lower effectiveness due to its filled d-orbital configuration, which limits redox interactions.

Minimum Inhibitory Concentration (MIC)

The Minimum Inhibitory Concentration (MIC) values were determined using the broth microdilution technique to quantify the antibacterial potency of the synthesized compounds. Lower MIC values indicate higher antibacterial effectiveness.

The Cu(II) complex exhibited the lowest MIC values against all bacterial strains, confirming its superior antimicrobial potency. The Ni(II) complex ranked second, followed by Co(II) and Zn(II). The free Schiff base ligand required considerably higher concentrations to inhibit bacterial growth, further confirming that complexation enhances biological activity.

Table 9. Minimum Inhibitory Concentration (MIC)

Compound	S. aureus (µg/mL)	B. subtilis (µg/mL)	E. coli (µg/mL)	P. aeruginosa (µg/mL)
Schiff Base Ligand	125	125	250	250
Cu(II) Complex	15.62	15.62	31.25	31.25
Co(II) Complex	31.25	31.25	62.50	62.50
Ni(II) Complex	15.62	31.25	31.25	62.50

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Compound	S. aureus (µg/mL)	B. subtilis (µg/mL)	E. coli (µg/mL)	P. aeruginosa (µg/mL)
Zn(II) Complex	62.50	62.50	125	125
Ciprofloxacin	3.90	3.90	3.90	3.90

The MIC values correlate well with the agar well diffusion results. Compounds exhibiting larger inhibition zones also showed lower MIC values, confirming the reliability of the antibacterial evaluation. The Cu(II) complex demonstrated the strongest bactericidal effect, requiring only a small concentration to inhibit microbial growth.

Structure–Activity Relationship (SAR)

The observed antibacterial activity of the synthesized compounds can be explained by considering the relationship between molecular structure and biological function. The Schiff base ligand contains an azomethine (–CH=N–) group and heterocyclic donor atoms capable of coordinating with transition metal ions. Upon complex formation, electron delocalization increases throughout the molecule, reducing the polarity of the metal ion and enhancing the lipophilic character of the complex.

According to Tweedy's Chelation Theory, increased lipophilicity improves the ability of the metal complex to penetrate bacterial lipid membranes. Once inside the bacterial cell, the complexes may interfere with essential metabolic pathways by binding to DNA, inhibiting protein synthesis, disrupting enzyme activity, and generating reactive oxygen species (ROS). These combined effects ultimately lead to bacterial cell death.

Among the investigated metal ions, Cu(II) possesses the highest biological activity due to its variable oxidation state and ability to participate in redox reactions that produce oxidative stress within bacterial cells. Nickel(II) and cobalt(II) complexes also exhibited strong antibacterial properties because of their stable coordination geometries and effective interaction with biomolecules. Zinc(II), although biologically important, displayed comparatively lower activity because of its redox-inactive d^{10} electronic configuration.

The presence of heterocyclic oxygen and nitrogen donor atoms further stabilizes the coordination sphere and enhances electron delocalization, contributing to the overall biological performance of the synthesized complexes.

Proposed Mechanism of Antibacterial Action

The antibacterial activity of heterocyclic Schiff base metal complexes is believed to involve several complementary mechanisms:

1. Increased lipophilicity facilitates penetration through the bacterial cell membrane.
2. Binding of the complex to bacterial DNA inhibits replication and transcription.
3. Interaction with essential enzymes blocks important metabolic processes.
4. Generation of reactive oxygen species (ROS) induces oxidative damage to cellular components.
5. Disruption of membrane integrity causes leakage of intracellular constituents.
6. Inhibition of protein synthesis ultimately results in bacterial cell death.

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These mechanisms collectively explain the superior antibacterial activity of the synthesized metal complexes compared with the free Schiff base ligand.

4. DISCUSSION

The present investigation successfully demonstrated the synthesis of heterocyclic Schiff base ligands and their coordination with Cu(II), Co(II), Ni(II), and Zn(II) ions. The synthesized compounds were obtained in good yields and exhibited excellent stability under laboratory conditions. Spectroscopic investigations, including FT–IR, UV–Visible spectroscopy, elemental analysis, magnetic susceptibility, molar conductance, and thermogravimetric analysis, consistently confirmed the successful formation of coordination complexes.

The FT–IR spectra confirmed coordination through the azomethine nitrogen and heterocyclic oxygen donor atoms, while UV–Visible spectroscopy and magnetic susceptibility measurements suggested predominantly octahedral geometries for the Cu(II), Co(II), and Ni(II) complexes. Low molar conductance values established the non-electrolytic nature of the synthesized compounds, and TGA revealed enhanced thermal stability following complexation.

Biological evaluation demonstrated that all synthesized metal complexes exhibited greater antibacterial activity than the free Schiff base ligand. The Cu(II) complex showed the highest activity against both Gram-positive and Gram-negative bacteria, followed by the Ni(II), Co(II), and Zn(II) complexes. The enhanced antibacterial properties can be attributed to increased lipophilicity, efficient membrane penetration, stronger interaction with intracellular biomolecules, and the ability of transition metals to induce oxidative stress within bacterial cells.

Overall, the findings confirm that coordination of heterocyclic Schiff bases with transition metal ions significantly improves their physicochemical stability and biological activity. These results suggest that such metal complexes represent promising candidates for the development of new antimicrobial agents capable of combating drug-resistant bacterial pathogens. Further investigations involving molecular docking, cytotoxicity studies, in vivo biological evaluation, and pharmacokinetic analysis are recommended to explore their therapeutic potential and possible pharmaceutical applications.

5. CONCLUSION

The present study successfully demonstrated the synthesis of a heterocyclic Schiff base ligand and its transition metal complexes with Cu(II), Co(II), Ni(II), and Zn(II). The synthesized compounds were obtained in good yields and exhibited excellent stability under laboratory conditions. Spectral characterization using FT–IR, UV–Visible spectroscopy, ^1H NMR, elemental analysis, molar conductance, magnetic susceptibility, and thermogravimetric analysis confirmed the successful formation of the Schiff base ligand and its coordination with the selected metal ions. The analytical results suggested that the ligand behaved as a bidentate donor through the azomethine nitrogen and heterocyclic oxygen atoms, forming stable coordination complexes with predominantly octahedral geometry. Biological evaluation revealed that all metal complexes exhibited enhanced antibacterial activity compared with the free Schiff base ligand, with the Cu(II) complex showing the highest inhibitory effect against both Gram-positive and Gram-negative bacterial strains. The improved

biological performance can be attributed to increased lipophilicity and stronger metal–ligand interactions after complexation. Overall, the findings indicate that heterocyclic Schiff base metal complexes are promising candidates for the development of new antibacterial agents. Further investigations involving molecular docking, cytotoxicity assessment, and in vivo pharmacological studies are recommended to explore their therapeutic potential and possible pharmaceutical applications.

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