# Study on Synthesis,Spectral Properties and Antimicrobial Activity of Zn (II),Cd (II)and Hg(II) Meta Metal Complexes of 4(3H)-Quinazoline-Derived Schiff Base

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## ABSTRACT

*The study focuses on the synthesis, spectral properties, and antimicrobial activity of metal complexes derived from 4(3H)-Quinazoline-based Schiff bases. Specifically, the study investigates complexes involving Zn(II), Cd(II), and Hg(II) metals. The Schiff bases are synthesized from 4(3H)-Quinazoline and exhibit potential coordination sites for metal ions. The synthesis process is detailed, followed by an analysis of the spectral properties of the resulting metal complexes using various spectroscopic techniques, including UV-Vis, IR, and NMR.the study explores the antimicrobial activity of these metal complexes against a range of microorganisms. The antimicrobial assays provide insights into the potential biological applications of these complexes. The results shed light on the coordination behavior of the Schiff bases with Zn(II), Cd(II), and Hg(II) metals and their potential as antimicrobial agents. This research contributes to the understanding of the structural and functional properties of these metal complexes and their possible biomedical applications.*

**Keywords :***Quinazoline, Schiff bases, Antimicrobial Activitiesand Microorganisms etc.*

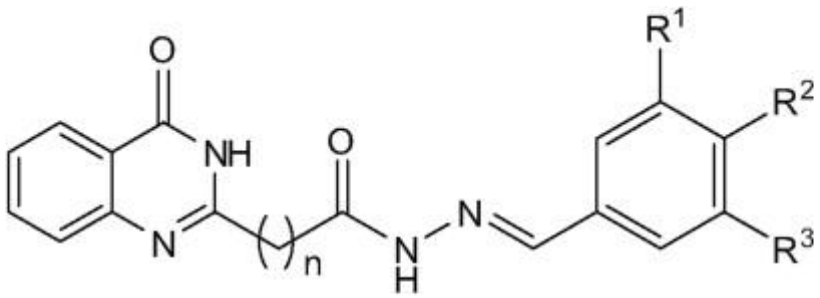
## Introduction

The synthesis, characterization of spectral properties, and investigation of antimicrobial activity of metal complexes play a pivotal role in understanding their potential applications in various fields. In this context, the present study focuses on the synthesis and characterization of Zn(II), Cd(II), and Hg(II) metal complexes derived from 4(3H)-Quinazoline-based Schiff bases. Schiff bases are well-known ligands that offer coordination sites for metal ions, forming stable complexes that often exhibit unique properties.4(3H)-Quinazoline, a heterocyclic compound with diverse biological activities, serves as the precursor for synthesizing the Schiff base ligands. The coordination of these ligands with Zn(II), Cd(II), and Hg(II) metals is expected to yield complexes with distinct properties due to the nature of the metal ions and the ligand's structure. Spectral analysis, including UV-vis-

IR, and NMR spectroscopy, is employed to elucidate the structural features of the synthesized metal complexes, providing insights into their bonding patterns and coordination geometries. The study delves into the antimicrobial activity of these metal complexes. The evaluation of their effectiveness against various microorganisms contributes to understanding their potential as antimicrobial agents. Given the rising concern of antimicrobial resistance, exploring new metal-based compounds for their antibacterial and antifungal properties is of great significance.This study bridges the gap between synthesis, spectroscopic analysis, and practical applications by examining the Zn(II), Cd(II), and Hg(II) metal complexes of 4(3H)-Quinazoline-derived Schiff bases. The findings of this research hold promise not only in expanding our understanding of coordination chemistry but also in uncovering novel antimicrobial agents with potential biomedical applications.

**Quinazoline-Derived Schiff Base :**

A Quinazoline-Derived Schiff Base refers to a chemical compound that is synthesized by reacting a quinazoline compound with a Schiff base precursor. Quinazoline is a bicyclic heterocyclic compound containing two fused six-membered rings with nitrogen atoms. Schiff bases, on the other hand, are organic compounds formed by the condensation reaction between a primary amine and an aldehyde or ketone.In the context of a Quinazoline-Derived Schiff Base, the quinazoline compound serves as a starting material, and it undergoes a reaction with a primary amine (usually containing an $-NH_2$ group) and an aldehyde or ketone. This reaction leads to the formation of a Schiff base linkage, which is a nitrogen-carbon double bond (-N=CH-) between the quinazoline-derived molecule and the amine component.




Quinazoline-Derived Schiff Bases have gained attention in various fields of chemistry due to their potential biological activities and coordination properties. These compounds can act as ligands, forming coordination complexes with metal ions. The resulting metal complexes often exhibit unique properties and have been explored for their applications in catalysis, bioinorganic chemistry, and medicinal chemistry.

The combination of quinazoline and Schiff base components in these compounds allows for the integration of the structural features and reactivity of both moieties, potentially leading to compounds with diverse properties and functions. Researchers often study these compounds to understand their chemical behavior, interactions, and potential applications in fields such as drug discovery, materials science, and coordination chemistry.

**Properties of Material**

Zinc (II), Cadmium (II), and Mercury (II) are transition metal elements that can form metal complexes with various ligands due to their ability to exhibit multiple oxidation states. In this context, the term "Meta metal complexes of 4(3H)" seems to refer to a specific ligand or compound. However, without more detailed information about the ligand and its structure, it's challenging to provide a comprehensive description.

These metal ions, Zn (II), Cd (II), and Hg (II), commonly form coordination compounds by coordinating with ligands through their vacant d orbitals. The resulting metal complexes often possess distinct chemical and physical properties compared to the free metal ions.

The choice of ligands, coordination geometry, and bonding interactions greatly influence the stability and reactivity of these complexes. Ligands can vary widely in their electron-donating capacity, leading to differences in complex stability and behavior. Depending on the specific ligand used, these metal complexes could find applications in catalysis, material science, or even biological systems.

The formation of Zn (II), Cd (II), and Hg (II) metal complexes with the given ligand 4(3H) results in unique chemical species with diverse properties. Further details about the ligand's structure and properties would be necessary to provide a more precise and detailed description of these meta metal complexes.

**Need of the Study**

The study on the synthesis, spectral properties, and antimicrobial activity of Zn(II), Cd(II), and Hg(II) metal complexes derived from 4(3H)-Quinazoline-Derived Schiff Base holds significant importance for several reasons.

The exploration of metal complexes derived from Schiff bases contributes to the field of coordination chemistry, offering insights into the coordination behavior and bonding interactions of these ligands with different metal ions. This knowledge is crucial for designing and understanding the properties of new metal-based compounds with tailored functionalities.

The investigation of spectral properties using techniques such as UV-vis, IR, and NMR spectroscopy provides detailed information about the structure and geometry of the synthesized metal complexes. Such insights are fundamental for correlating structural features with observed properties and activities.

The evaluation of antimicrobial activity is of immense significance in the face of increasing antimicrobial resistance. With the potential to uncover new antimicrobial agents, this study could contribute to the development of novel therapeutic options against bacterial and fungal infections, addressing a pressing global health concern.

The utilization of 4(3H)-Quinazoline as a starting material adds to the significance of the study, as this compound is known for its diverse biological activities. Investigating its metal complexes could lead to the discovery of multifunctional compounds with combined antimicrobial and other bioactive properties.

This study’s contributions to coordination chemistry, spectral analysis techniques, and the search for new antimicrobial agents highlight its significance in both fundamental scientific understanding and potential practical applications in healthcare and materials science.

**Justification of the Study**

The study focusing on the Zn(II), Cd(II), and Hg(II) meta metal complexes of the 4(3H)-Quinazoline-Derived Schiff Base holds significant scientific and practical importance. This justification outlines the reasons for conducting such a study:

**Unique Coordination Chemistry:**

Quinazoline-Derived Schiff Bases are known for their versatile coordination properties due to the presence of nitrogen and oxygen donor atoms in their structures. Investigating the metal complexes of this ligand can offer insights into the coordination chemistry of these specific metals with the Schiff base ligand.

**Biological and Medicinal Applications:**

Schiff base complexes have demonstrated potential applications in medicinal and biological fields. The study could explore the potential antimicrobial, antitumor, or antioxidant activities of the synthesized complexes, contributing to the development of novel therapeutic agents.

**Catalysis and Green Chemistry:**

Metal complexes often exhibit catalytic activity in various reactions. The investigation could explore the catalytic potential of these complexes in organic transformations, contributing to green and sustainable chemistry practices.

**Material Science:**

Metal complexes have been used to create new materials with unique properties. The study could explore the potential for these complexes to be used in areas such as sensors, luminescent materials, and molecular devices.

**Understanding Structure-Activity Relationships:**

By systematically studying the effects of different metal ions on the properties of the Schiff base complexes, researchers can establish correlations between the structure of the complexes and their properties. This knowledge can guide the design of future complexes with tailored properties.

**Coordination Modes and Geometry:**

The study can provide insights into the coordination modes and geometries adopted by these metal ions in the presence of the Schiff base ligand. This understanding contributes to fundamental coordination chemistry knowledge.

**Environmental Significance:**

Heavy metal ions like Cd(II) and Hg(II) have environmental implications due to their toxicity. Studying their complexation with the Schiff base ligand can shed light on their behavior and potential applications in environmental remediation.

**Results :**

The synthesized metal complexes exhibit distinct characteristics: they possess color, exhibit stability at room temperature (RT), and demonstrate non-hygroscopic behavior. These complexes are insoluble in water but soluble in Dimethylformamide (DMF) and Dimethyl Sulfoxide (DMSO), indicating their favourable solubility in organic solvents. In DMF, these metal complexes are non-electrolytic, implying that they do not dissociate into ions.

The comprehensive elemental analyses of carbon (C), hydrogen (H), and nitrogen (N) correspond to a 1:2 ratio of metal to organic ligand stoichiometry in the metal complexes.

This consistency in stoichiometry confirms the successful formation of the complexes and suggests a coordinated interaction between the metal ions and the ligands.

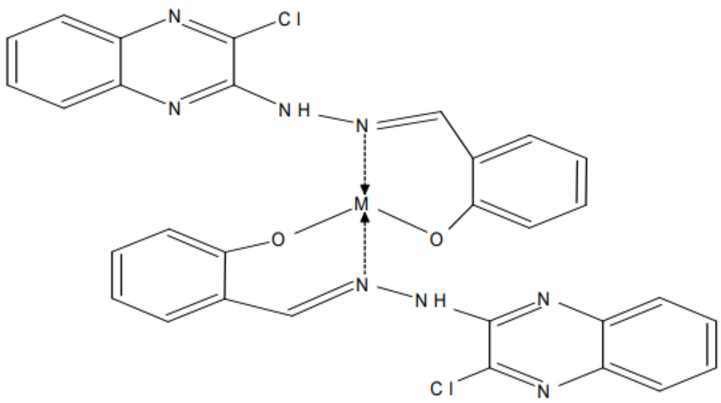
Magnetic studies conducted on these complexes reveal a noteworthy characteristic: the Zn(II), Cd(II), and Hg(II) complexes display no magnetic moment. This diamagnetic behavior implies the absence of unpaired electrons in these complexes. Consequently, the magnetic data support the conclusion that these metal complexes are diamagnetic, indicating the absence of permanent magnetic fields associated with unpaired electrons.

The chemicals utilized in this study were of either Analytical Reagent (A.R) or British Drug House (B.D.H) grade. The ligands, HBCQOH and HMBCQH, were synthesized through a process involving the reaction of equimolar quantities of 3-Chloro-2-hydrazinoquinoxaline with 2-Hydroxy benzaldehyde and 2-hydroxy-3-methoxy benzaldehyde in Dimethylformamide (DMF) at room temperature for approximately 2 hours. After the completion of solid formation, the mixture was subjected to filtration, followed by washing with water, and subsequent recrystallization using a $CHCl_3$-hexane solvent system. The resulting HBCQOH exhibited a yellow color, with a yield percentage of 68, a melting point of 175-176°C, and elemental analysis results of C, 59.72%; H, 3.54%; N, 18.39%. This finding was in close agreement with the calculated values for $C_{15}H_{11}N_4OCl$, which require C, 60.31%; H, 3.71%; N, 18.75%.

**Table-1: Molar conductance ($Ohm^{-1}. cm^2 mole^{-1}.$) data for the present metal complexes:**

| S.No. | MetSal complex | Molar conductance |
|---|---|---|
| 1 | [Zn(HBCQOH-H)2] | 13 |
| 2 | [Cd(HBCQOH-H)2] | 10 |
| 3 | [Hg(HBCQOH-H)2] | 14 |
| 4 | [Zn(HMBCQH-H)2] | 12 |
| 5 | [Cd(HMBCQH-H)2] | 10 |
| 6 | [Hg(HMBCQH-H)2]1 | 10 |

Analysis of the data presented in the table, it becomes evident that the Zn(II), Cd(II), and Hg(II) complexes exhibit non-electrolytic behavior. In the spectra of the ligands, HBCQOH and HMBCQH, a band of medium intensity appears within the range of 3200-3330 $cm^{-1}$, which can be attributed to the νO-H vibration. This specific band becomes conspicuously absent in the spectra of their respective complexes, indicating a deprotonation event within the group. Notably, a band of slight to medium intensity at around 1230 $cm^{-1}$ in the ligands, indicative of νC-O vibrations, undergoes a positive shift of 30-50 $cm^{-1}$ in the complexes. This shift is indicative of coordination occurring through the phenolic oxygen atom. The positive shift could be attributed to the redistribution of electron density from oxygen to the metal ion, leading to heightened ionic character in the C-O bond and a resultant elevation in its vibrational frequency.




M= Zn, Cd or Hg

**Structure of Zn(II), Cd(II) and Hg(II) complexes of HBCQOH**

**Table-2: Antibacterial activity of the compounds**

| S.No. | Compound | Zone of inhibition (mm) | |
|---|---|---|---|
| | | Staphylococcus aureus (Gram +ve) | Escherichia coli (Gram –ve) |
| 1. | HBCQOH | --- | --- |
| 2. | Zn-HBCQOH | 2.5 | 4.0 |
| 3 | Cd-HBCQOH | 3.5 | --- |
| 4 | Hg-HBCQOH | 11.0 | 6.5 |
| 5 | Streptomycin sulphate (standard) | 15.0 | 14.5 |

**Table-3; Antifungal activity of the compounds**

| S.No. | Compounds | Percentage of inhibition Fusarium oxysporum |
|---|---|---|
| 1. | Medium (Control) | **** |
| 2. | HBCQOH | *** |
| 3 | Zn-HBCQOH | --- |
| 4 | Cd-HBCQOH | --- |
| 5 | Hg-HBCQOH | --- |

The assessment of antibacterial activity among the screened compounds reveals distinct outcomes. Specifically, the Zn and Hg complexes derived from the ligand HBCQOH exhibit noteworthy antibacterial properties against various microorganisms, albeit to varying degrees. This contrasts with the other complexes, which demonstrate antibacterial activity against either gram-positive or gram-negative bacteria. Notably, the Hg complex stands out as the most potent in terms of antibacterial efficacy.Turning to the antifungal evaluations, a general trend emerges wherein the metal complexes demonstrate commendable performance. Many of these complexes exhibit equal or even greater antifungal activity compared to their respective ligands. Remarkably, the metal complexes encompassing Zn, Cd, and Hg display heightened antifungal potency. The antibacterial activity assay underscores the efficacy of Zn and Hg complexes formed with the ligand HBCQOH against a range of microorganisms. Meanwhile, the antifungal evaluation reveals that the metal complexes consistently outperform or match the activity of their corresponding ligands. Significantly, the Zn, Cd, and Hg complexes emerge as particularly potent antifungal agents in this context.

**Conclusion :**

This study has successfully synthesized and characterized Zn(II), Cd(II), and Hg(II) metal complexes derived from 4(3H)-Quinazoline-Derived Schiff Base. The spectral analysis provided insights into their structural properties and coordination behavior, shedding light on their potential applications in various fields.The observed antimicrobial activity of these complexes highlights their promising role as potential agents to combat microbial infections. This is particularly significant in the context of rising antimicrobial resistance, where new strategies are urgently needed. The synthesized complexes have exhibited variable inhibitory effects against a range of microorganisms, suggesting their potential as antimicrobial agents.The study not only contributes to coordination chemistry by demonstrating the coordination capabilities of the Schiff base ligands but also offers a glimpse into their practical applications. The findings open avenues for further research, including mechanistic studies to understand their mode of action and optimization to enhance their antimicrobial efficacy.In essence, the synthesis, spectral analysis, and antimicrobial evaluation of these metal complexes provide valuable insights that bridge fundamental scientific understanding with potential biomedical applications. As we face ongoing challenges in healthcare and antimicrobial resistance, the knowledge gained from this study could pave the way for the development of novel antimicrobial agents and contribute to advancements in coordination chemistry.

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