SYNTHESIS, CHARACTERIZATION, MOLECULAR MODELLING AND BIOACTIVITY STUDIES OF COBALT, NICKEL, COPPER AND ZINC COMPLEXES WITH TETRADENTATE SCHIFF BASES

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A thesis submitted in fulfilment of the
requirements for the award of the degree of
Doctor of Philosophy (Chemistry)

Faculty of Science
Universiti Teknologi Malaysia

JANUARY 2023

DEDICATION

This thesis is wholeheartedly dedicated to my father, mother and the late Yammoi and Hotine that had left me in August. I lost half of my soul. This journey is very challenging, that certainly needs self-effort and guidance from the elders. Their affection, love, encouragement, support, endless prayers days and nights have made me strong to endure all these.

They are my pillar of strength.

ACKNOWLEDGEMENT

Alhamdulillah, all praises and thanks to ALLAH SWT for His showers of blessing throughout my research work, to complete this research successfully.

It is a genuine pleasure to express my deep sense of thanks and gratitude to my supervisor, mentor, my guide and pathfinder, Prof. Dr. Mustaffa Shamsuddin for his dedication and wisdom throughout this project, from inception to completion. His unwavering patience, as well as scholarly advice, have helped me to a very great extent in completing this task.

A profound sense of gratitude also goes to Assoc. Prof. Dr Ku Halim Ku Bulat for his invaluable mentoring, overwhelming support, and guidance especially in theoretical chemistry. His prompt inspirations, timely suggestions with kindness and enthusiasm have enabled me to complete my thesis. I feel very lucky to have both as my mentors. I shall be forever obliged to their guidance. They are my backbone in moulding my academic enhancement. May Allah bless them with good health, peace, happiness and allocate them a place in Jannah.

I would also like to express my sincere thanks to Prof. Dr. Noraznawati Ismail, the biologist expert who had been involved in evaluating the potential of antibacterial activity. I was given a chance to work in her microbe lab, with the assistance of her research students. Her constructive comments and suggestions have contributed to the success of this research.

No words of thanks can sum up my gratitude to my parents for their prayers, love, constant encouragement, and sacrifices for educating and preparing me for the future. I am also very thankful to my colleagues and friends that I had incredible joy and pleasure of working with. It was very pleasant to befriend with Dr. Faraidoon and his wife, Tavan, Dr. Suhaila, Nur Hafizah and Madam Fazleen, just to name a few. Also, I thank profusely all the staffs of Department of Chemistry, UTM for their kind help and cooperation throughout my study period.

Personally, I would like to thank my best friend, Afiq for always be there for me through thin and thick. Also, thanks to Dr Ku's team, Miss Radiah and Madam Isrina for their help, suggestions, and willingness to answer questions even at night to diminish my worries over computational problems. Thanks to Dr. Noor Azniza for her helping hand, offering friendship, and accommodations while I was in Terengganu for my attachment. Honestly, I am indebted to everyone I met along the way in this journey, nevertheless good or bad, you have taught me a valuable lesson that I am not able to forget. Thank you.

ABSTRACT

The search for new active antimicrobial compounds is of growing interest since the current antibiotics remain insufficient to tackle the challenge of increasing emergence and spread of antimicrobial resistance. Inorganic compounds particularly metal complexes have played an important role in the development of new metal-based drugs. In this regard, there is a strong need to synthesize new compounds that possess good chemical reactivity and are comprehensively studied with the help of theoretical calculation. In this study, four types of Schiff base ligands have been synthesized by the condensation between 2,4-dihydroxyacetophenone and appropriate amines in a 2:1 molar ratio. Mononuclear Ni(II), Cu(II), Co(II) and Zn(II) metal complexes were prepared and characterized by elemental analysis, molar conductivity, Ultraviolet-Visible, infrared and nuclear magnetic resonance spectroscopies as well as single crystal X-ray diffraction analysis. Spectral data revealed that the ligand acted as O,N,N,O tetradentate chelating to the metal ion through phenolate oxygen and azomethine nitrogen atoms. The geometry of the ligands and the metal complexes were optimized by Density Functional Theory (DFT) using Gaussian 09 software package at theoretical level B3LYP/6-311G++(d,p) for ligands and B3LYP/GEN for metal complexes. The experimental results were corroborated by the calculations data. All compounds were subjected to antibacterial activities against two gram-positive and two gram-negative bacterial strains. All the compounds showed broad spectrum of antibacterial activities. Co(II) complexes were generally active against both gram-positive and gram-negative bacteria with minimum inhibitory concentration (MIC) values ranging from 0.02 to 5 mg/mL. The results showed that metal chelation contributes to significant antibacterial activities. The antioxidant potentials of the compounds were evaluated using 2,2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging assay. The ligands had higher antioxidant potentials compared to metal complexes. However, some phenylene-containing complexes exhibited excellent scavenging activity with their SC_{50} values ranging from 11.3 to 79.9 μg/mL.

ABSTRAK

Pencarian sebatian antimikrob aktif baharu semakin berkembang kerana antibiotik terkini masih tidak cukup untuk menangani cabaran peningkatan kemunculan dan rebakan kerintangan antimikrobial. Sebatian bukan organik khususnya kompleks logam telah memainkan peranan penting dalam pembangunan ubat berasaskan logam baharu. Justeru itu terdapat keperluan mendesak untuk mensintesis sebatian baharu yang mempunyai kereaktifan kimia yang baik dan dikaji secara menyeluruh dengan bantuan pengiraan teoritikal. Dalam kajian ini, empat jenis ligan bes Schiff telah disintesis melalui kondensasi antara 2,4-dihidroksiasetofenon dan amina yang bersesuaian dalam nisbah molar 2:1. Kompleks logam mononuklear Ni(II), Cu(II), Co(II) dan Zn(II) telah disediakan dan dicirikan menggunakan analisis unsur, kekonduksian molar, spektroskopi ultra-lembayung nampak, inframerah dan resonans magnet nukleus serta analisis pembelauan sinar-X hablur tunggal. Data spektrum memperlihatkan ligan bertindak sebagai tetradentat O,N,N,O terkelat kepada ion logam melalui oksigen fenolat dan atom nitrogen azometin. Geometri ligan dan kompleks logam dioptimumkan dengan menggunakan pakej perisian Gaussian 09 pada tahap teori fungsi ketumpatan (DFT) B3LYP / 6-311G ++ (d, p) bagi ligan dan B3LYP/GEN bagi kompleks logam. Keputusan eksperimen telah disokong oleh data pengiraan. Semua sebatian telah diuji aktiviti antibakteria terhadap dua jenis bakteria gram-positif dan dua jenis bakteria gram-negatif. Semua sebatian menunjukkan aktiviti antibakteria yang luas spektrumnya. Secara umum kompleks Co(II) adalah aktif terhadap kedua-dua bakteria gram-positif dan gram-negatif dengan nilai perencatan minimum (MIC) dari julat 0.02 hingga 5 mg/mL. Keputusan menunjukkan pengkelatan logam menyumbang kepada aktiviti antibakteria yang lebih signifikan. Potensi antioksidan sebatian telah dinilai menggunakan cerakin pemerangkapan radikal 2,2-difenil-1-pikrilhidrazil (DPPH). Ligan mempunyai potensi antioksidan yang lebih tinggi berbanding dengan kompleks logam. Walau bagaimanapun, beberapa kompleks yang mengandungi fenilena menunjukkan aktiviti pemerangkapan yang sangat baik dengan nilai SC_{50} dalam julat 11.3 hingga 79.9 μg/mL.

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LIST OF ABBREVIATIONS

AMR	-	Antimicrobial Resistance
WHO	-	World Health Organization
^{1}H-NMR	-	Proton Nuclear Magnetic Resonance
^{13}C-NMR	-	Carbon-13 Nuclear Magnetic Resonance
IR	-	Infrared
UV-Vis	-	Ultraviolet-Visible
DMSO	-	Dimethyl Sulphoxide
DMSO-d_6	-	Deuterated dimethyl sulphoxide
DFT	-	Density Functional Theory
TD-DFT	-	Time Dependant Density Functional Theory
B3LYP	-	Becke 3-parameter Lee-Yang-Parr
UB3LYP	-	Unrestricted Becke 3-parameter Lee-Yang-Parr
CAM-B3LYP	-	Coulomb-attenuating Method Becke 3-parameter Lee-Yang-Parr
LANL2DZ	-	Los Alamos National Laboratory 2 Double-Zeta
GEN	-	General
NBO	-	Natural Bond Orbital
MEP	-	Molecular Electrostatic Potential
ESP	-	Electrostatic Potential
PCM	-	Polarizable Continuum Model
HOMO	-	Highest Occupied Molecular Orbital
LUMO	-	Lowest Unoccupied Molecular Orbital
WLS	-	Wavenumber Linear Scaling
ED	-	Electron Density
PED	-	Potential Energy Distribution
VEDA	-	Vibrational Energy Distribution Analysis
GIAO	-	Gauge-Independent Atomic Orbital
TMS	-	Tetramethylsilane
IEF-PCM	-	Integral-Equation-Formalism Polarizable Continuum Model

NLO	-	Nonlinear Optical
def2-TZVP	-	Valence Triple-Zeta with two sets of Polarization functions
PBE	-	Perdew–Burke-Ernzerhof
pVTZ	-	polarised Valence Triple Zeta
DN	-	Double Numerical
DNP	-	Double Numerical Polarization
GGA	-	Generalised Gradient Approximation
B3P86	-	Becke 3-part functional; Perdew correlation 1986
TGA/DTA	-	Thermogravimetric Analysis/ Differential Thermal Analysis
TGA/DSC	-	Thermogravimetric Analysis/Differential Scanning Calorimetry
SEM	-	Scanning Electron Microscope
XRD	-	X-ray Powder Diffraction
ESI-MS	-	Electrospray Ionization-Mass Spectrometry
DNA	-	Deoxyribonucleic Acid
LMCT	-	Ligand to metal charge transfer transition
DPPH	-	1,1-diphenyl-2-picrylhydrazyl
MIC	-	Minimum Inhibition Concentration
SC_{50}	-	Scavenging Concentration at fifty percent
Cpd	-	Compound
SD	-	Standard Deviation
r.t.	-	room temperature
HCT116	-	Human Colorectal Carcinoma

LIST OF SYMBOLS

nm	-	nanometer
π	-	pi
n	-	non bonding
°C	-	degree celcius
cm^{-1}	-	reciprocal wavelength
λ	-	wavelength
mL	-	mililiter
%	-	percentage
mmol	-	milimole
g	-	gram
mg	-	miligram
μg	-	microgram
ρ	-	density
M	-	molarity
mM	-	milimolar
μM	-	micromolar
ε	-	molar absorptivity
Λ_M	-	molar conductance
°	-	degree angle
Å	-	angstrom
a.u	-	atomic unit

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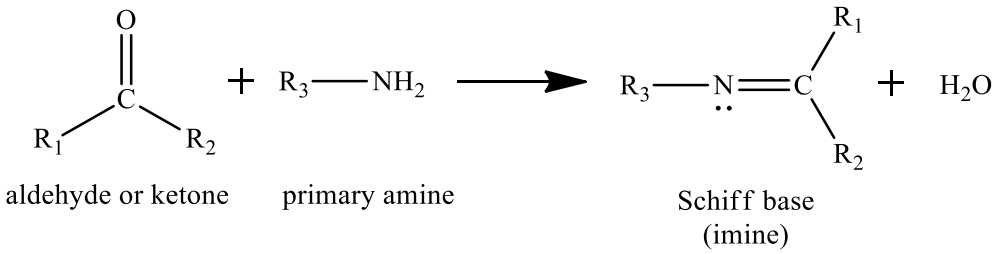
CHAPTER 1

INTRODUCTION

1.1 Research Background

Schiff base is a compound with general structure R_1─CR_2=N─R_3, where R_1, R_2 and R_3 could be H, linear or cyclic alkyl and/or aryl group ($R_3 \neq H$) which may be differently substituted (Scheme 1.1) [1]. Schiff bases also known as imines and are typically formed from the condensation reaction between primary amine with carbonyl compounds either ketone or aldehyde. Schiff bases are an important class of ligands for coordination chemistry, and they coordinate to metal ions *via* the imine or azomethine nitrogen. Schiff base ligands have been comprehensively studied in the field of coordination chemistry mainly due to their facile syntheses, easy availability, and interesting electronic properties [2-4]. Moreover, the coordination chemistry of Schiff base has drawn remarkable attention because of their significance in catalysis, analytical chemistry, dye industry and metallurgy [3, 5, 6]. Additionally, the Schiff base's azomethine linkage (–C=N) is an essential structural requirement for biological activities. Several Schiff bases and their transition metal complexes are reported to possess remarkable antibacterial, antifungal, and anticancer activities [7-10].



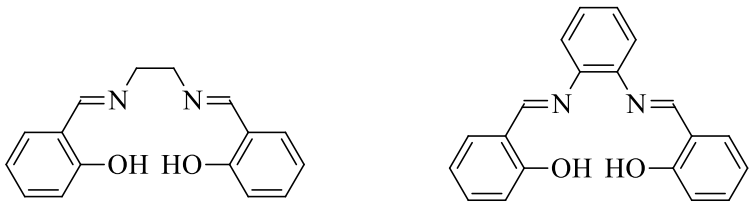
R_1, R_2 and/or R_3 = H, alkyl or aryl (R_3 is not equal to H)

Scheme 1.1 General scheme for formation of Schiff base [1]

The main characteristic of Schiff base ligand is the presence of the imine group (-RC=N-). The metal complex formation takes place by coordinating through the imine nitrogen, which provides a site for complexation. Due to its tuneable electronic properties, Schiff base is also able to stabilize different metals in various oxidation states. Hence, they are suitable to control the metals' performance in numerous organic catalytic transformation reactions [11-13]. In addition, Schiff base ligands are stable at ambient temperature towards air and moisture attack. Literally, the ease of synthesizing Schiff bases and their interesting and tuneable electronic properties have stimulated the growth of structural design of molecules to be utilized in biochemistry, material sciences, catalysis, hydrometallurgy and separation science [14-16].

The chemistry of Schiff base ligands and their metal complexes have expanded exceptionally and encompassed a vast area of coordination and organometallic compounds. They gained attention due to their chelation ability to metal ions, which significantly increased when introduced to donor atoms' strategic positions in the molecule. Thus, it has allowed a massive array of metal complexes with compelling structural architectures [17, 18].

Among the various Schiff bases, more attention has been put on a class of Schiff base known as 'Salen'. The Salen-type Schiff base is derived from the condensation of two equivalents of salicylaldehyde and a diamine (Figure 1.1). The general term Salen-type is utilized in order to represent the class of [O, N, N, O] tetradentate bis-Schiff base ligands [19].



Salen Salophen

Figure 1.1 The molecular structures of Salen and Salophen

Salen and salophen have been widely studied in the medicinal field to act as antibacterial, antifungal, anticancer, antioxidants as well as other biological applications [18, 20, 21]. Salen and salophen ligands are generally multidentate ligands capable of forming complexes with transition metals. The chelating behaviour of the Schiff base plays an essential role in connections with their biological potential. This type of Schiff base's chemical stability can be achieved through complexation of transition metal through nitrogen and oxygen donor atoms. Upon coordination, the possibility of the metal to have various oxidation states has led to important function in enzymatic redox system and bioinorganic chemistry which may provide the biologically active system [22]. Therefore, the biological activity of the compound is greatly influenced by the presence of metal ions as mentioned in previous reports [23-26]. Schiff base contributes to the geometrical cavity control for host-guest interaction. Besides, it helps in modulating lipophilicity that offers remarkable selectivity, sensitivity as well as stability towards a specific metal ion [15]. Apparently, Schiff base complexes with ONNO donor atoms are suitable for studies in the modelling of bioinorganic processes [27].

For a comprehensive understanding of the structural-activity relationship, utilization of quantum chemical calculations and spectroscopic characterization has attracted a significant amount of interest [28-30]. By employing computational chemistry, it helps to complement the information acquired by experiment and provide deeper insight in terms of interaction energies and exchange of energies in a molecular system [31, 32].

Indeed, for the past 30 years, density functional theory (DFT), introduced by Kohn and John People [33-35] has evolved and used as a vital tool in many chemistry branches. One of the most interesting features of quantum chemical calculations is the electronic simulations of atoms and molecules [36]. Hence, DFT aims to predict materials' behavior with anticipated potential as the sum of external potential due to structure and composition of material as well as effective potential owing to inter electronic interaction [37].

With the perfect combination of method, basis set and calculation level, a systematic calculation of the studied system can be achieved. Furthermore, the molecular orbital calculation enables to understand, help in molecular architecture, and predict the structure related activity of a compound with accuracy. The investigated parameters that dependent on the structure and geometry are bond lengths, bond angles, dipole moment, molecular energies, transition probabilities, vibrational studies which are the vital aspects to give a comprehensive understanding of a molecular system.

1.2 Problem Statements

The application of metal ions in the medical field started with organometallic complex of arsenic for the syphilis treatment [38], gold complex for rheumatoid arthritis treatment [39], and the platinum-based anti-cancer drugs namely, cisplatin, oxaliplatin and carboplatin [40]. Despite their immense potential as a treatment for certain diseases, their antimicrobial properties tend to be overlooked. The diversification of metals, ligands and the conformation of geometries have generated versatile metal-based complexes that able to fit in the field of drug development especially for the design of antimicrobials targeted compounds. Therefore, the development of new antimicrobial agents based on metal complexes have been actively investigated and expected to tackle the spread of antimicrobial resistance (AMR).

Schiff base ligand and their metal complexes possess huge potential to be studied thoroughly. Although numerous examples of Schiff base metal complexes have been considered for their remarkable antimicrobial activity, these findings are still inadequate, and discovery of new potential compounds with enhanced antibacterial properties are still essential.

Additionally, fewer reports have been published on the biological properties of Schiff base ligand especially in salen and salophen metal complexes. These Schiff base ligands are expected to bind with four donor atoms, N, N, O, and O atoms, to act as

tetradentate ligands. Higher coordination and chelation ability are believed to provide further stabilities for metal complex formation. Due to that fact, greater results and higher potential are expected on their biological activities by complexation with the *d*-block metals [41].

Even though Schiff base type ligands have been continually investigated, however, the available information is insufficient and most of the previous research studies only focused on experimental works. Literature reviews revealed that no theoretical studies were made on the exact molecular structures of salen and salophen. In addition, even though almost similar structures were reported theoretically, they utilized different basis set and different parameters measured. Hence, in the present research, attempts were made to synthesize the Schiff base and their respective Co(II), Ni(II), Cu(II) and Zn(II) complexes. The investigations in terms of their spectroscopic properties were both performed experimentally and theoretically. All compounds were then subjected to the evaluation of their antibacterial and antioxidant properties. The quantum chemical calculations in this study were performed using Gaussian 09 software package [42] with gas phase B3LYP calculation methods [43].

1.3 Research Objectives

The objectives of this research can be summarized as follows:

a) To synthesize and characterize the Schiff base and their corresponding Co(II), Ni(II), Cu(II) and Zn(II) complexes derived from the condensation of 2,4-dihydroxyacetophenone with ethylenediamine, phenylenediamine, 1,3-diaminopropane and 2,2-dimethyl-1,3-diaminopropane.
b) To perform the density functional theory (DFT) calculations on all synthesized ligands and complexes.
c) To explain the structural and spectral characteristic of the synthesized ligands and complexes based on experimental and theoretical findings.
d) To evaluate the antibacterial and antioxidant activities of the prepared ligands and their metal complexes.

1.4 Scope of Research

This research focused on the preparation of Schiff base derived from the condensation of 2,4-dihydroxyacetophenone with ethylenediamine, phenylenediamine, 1,3-diaminopropane and 2,2-dimethyl-1,3-diaminopropane. Complexation of these ONNO donor set Schiff bases was performed with selected metal ions such as Co(II), Ni(II), Cu(II) and Zn(II). All the prepared ligands and their related metal complexes were characterized by various typical spectroscopic techniques such as fourier transform infrared (FTIR) spectroscopy, ultraviolet-visible (UV-Vis) spectroscopy, ^{1}H nuclear magnetic resonance (NMR) spectroscopy, carbon, hydrogen, and nitrogen (CHN) elemental analysis as well as single crystal X-ray diffraction analysis.

Furthermore, the structures of ligands and metal complexes were drawn using Gaussview 5.0 and theoretically calculated using Gaussian 09 software package on a personal computer. The structure was optimized individually, and the optimized structural parameters were then used to calculate the spectroscopic including the theoretical spectrum of IR, UV-Visible, and ^{1}H NMR. Besides, the calculation also enabled finding the local minima, analysing the natural bond orbital (NBO), and determining physicochemical properties for instance, frontier molecular orbital and molecular electrostatic potential map.

Finally, the performance of all the prepared ligands and their corresponding Co(II), Ni(II), Cu(II) and Zn(II) complexes were tested for their biological activities. The antibacterial activity were conducted against two Gram-positive (*Staphylococcus aureus* ATCC 29523 and *Staphylococcus epidermidis* ATCC 13518) and two Gram-negative (*Escherichia coli* ATCC 11775 and *Salmonella typhi* ATCC 14128) bacterial strains. The bacteria inhibition was measured in terms of inhibition zone. Meanwhile, the antioxidant activity against DPPH radical scavenging assay was determined with reference to scavenging concentration at 50% of radical scavenging assay (SC_{50} µg/mL).

1.5 Significance of Research

Generally, Schiff base type ligand has been widely recognized and acknowledged due to their ease of synthesis, air stability and relatively cheap starting materials. The rapidly growing interest in synthesizing Schiff base has gained remarkable attention due to their structural flexibility, form stable complexes with many transition metal ions and considered as convenient synthetic block due to their chelating properties. Even though salen and salophen have been reported since the last few decades, but the studies of the complete molecular structures of salen and salophen seem limited. Few reports were made on their spectroscopic characterizations and screening their potential in any of biological activities. Besides, with the current interest in exploring theoretical aspects of a structure, utilization of DFT seems a favourable tool in order to help in gaining extensive understanding about the interaction of electron and nuclei in the studied system. As a result, the combination of experimental and theoretical correlation is definitely giving a bigger picture of a molecule's system and able to explore the fundamental aspect of chemistry.

In this work, the pharmacological effect of Schiff base and metal complexes is reviewed. The expanding field of bioinorganic chemistry has demanded therapeutic and diagnostic properties of metal complexes which are effective in treating disease and possess less toxic side effects. This is because, until now, very less metallodrugs reach the clinical trials stage due to lack of public acceptance and toxicity related issues that associated with the presence of metals. The slow rate of new drug development has also triggered researchers to explore and promote the growth of antimicrobial metallodrugs as a promising strategy to overcome the global rise of AMR.

Additionally, the synthesized ONNO organic ligands and their complexes of Co(II), Ni(II), Cu(II) and Zn(II) offered a beneficial and considerable biological applications especially for antibacterial and antioxidant activities due to the chelation effect. The wide range of metals and combination of various types of ligands are essential to adjust the lipophilicity of the metal complex, as it could contribute to their penetration ability of the cell membrane and thus, giving a substantial impact on biological activities.

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LIST OF PUBLICATIONS

Journal with Impact Factor

1. **Falynee Faha Abdul Wahab**, Mustaffa Shamsuddin, Ku Halim Ku Bulat and Noraznawati Ismail. (2018). Structural, Density Functional Computational Studies and Antibacterial Screening on *N,N'*-bis-(4-hydroxy-α-methylsalicylidene)ethylenediamine Nickel(II) complex. *Polyhedron*. *156*, 165-173. https://doi.org/10.1016/j.poly.2018.09.016. **(Q2, IF: 3.052)**

Non-indexed Conference Proceedings

1. Falynee Faha Abdul Wahab, Mustaffa Shamsuddin and Ku Halim Ku Bulat. Synthesis, Structural and Computational Studies of *N,N'*-bis-(4-hydroxy-α-methylsalicylidene)ethylenediamine. *Paper presented at 19th Malaysian International Chemistry Conference (19MICC) 2018.* October 30th – November 2nd. Bayview Hotel, Langkawi.

2. **Falynee Faha Abdul Wahab**, Mustaffa Shamsuddin and Abdul-Hamid Alizadeh. The Novel Triazine Cored mono-, di-, tri- podal ligands: From Synthesis to Application. *Paper presented at Regional Annual Fundamental Science Symposium 2014.* September 8th-11th. Persada Johor International Convention Centre, Johor Bharu.