

*Dedicated*  
*to*  
*The Almighty God and my beloved family*

## Declaration

I hereby declare that the thesis titled "**Exploration of the Chelation Property of few newly designed (N,O)-type Schiff base ligands with d-block metals and Bio-oxidase activities of their synthetic Coordination Compounds**" submitted for the award of Ph.D. degree represents my original research conducted at the Department of Chemistry, University of North Bengal. I conducted this research under the supervision of Professor Bhaskar Biswas. Additionally, I confirm that this thesis has not been used as the basis for the award of any other degree prior to this.

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## CERTIFICATE

I certify that under my guidance, Ms. Shreya Mahato has conducted her research work on "Exploration of the Chelation Property of few newly designed (N,O)-type Schiff base ligands with d-block metals and Bio-oxidase activities of their synthetic Coordination Compounds" at the Department of Chemistry, University of North Bengal, and is now eligible for the award of Ph.D. degree from the same university.

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Exploration of the Chelation Property of few newly designed (N,O)-type Schiff base ligands with d-block metals and Bio-oxidase activities of their synthetic Coordination Compounds Thesis Submitted to University of North Bengal in partial fulfilment of the requirements for the degree of Doctor of Philosophy in Chemistry By Ms. Shreya Mahato (M.Sc. in Chemistry) Supervised by Prof. Bhaskar Biswas Department of Chemistry University of North Bengal Darjeeling-734013 West Bengal, India May 2023

1 Chapter I General Introduction The revelation of the close connection between biology and inorganic chemistry gave birth to a distinct discipline called bioinorganic chemistry. The employment of superior spectroscopic tools and revolutionary high-resolution image-processing instruments flourished in this field. New and fascinating interdisciplinary research are being done since then. Especially, the role of metal ions in this field is undeniable. Metal ions are essential for the nourishment of life and can be considered as the protagonist in various biochemical reactions, playing structural and functional roles. The specificity of any metal ion for a particular biological process depends upon factors like valency, redox property, coordination plasticity, ligand affinity, etc. Metal ions having tunable redox properties like Fe, Co, Mn, Ni, Cu, and redox inactive ones like Zn, Ca, Mg, Na, and K are commonly employed in biological systems. For example, metalloprotein in photosynthesis [1], respiration [2], oxygen transport both in vertebrates [3] and invertebrates [4], and biocatalysts like nitric oxide reductases [5], hydrogenase [6], nitrogenase [7,8], superoxide dismutase [9,10], and many other engage metals to carry out their respective functionality. In addition, Metal complexes constitute a significant category of compounds with diverse applications across multiple fields. The scientific literature on this topic is vast and constantly growing to uncover new applications and properties of these fascinating compounds. Their incorporation in different ailments ranging from microbial infections to cancer treatment is noteworthy. [11-16] However, the journey from their discovery to commercialization is a time-consuming process and goes through a series of regulatory hurdles to get government approval. Therefore, the judicious designing of metallo-therapeutics remains a challenging task for bioinorganic chemists. Literature survey suggests that the ability of metal complexes to activate and stabilize reactive intermediates makes them a perfect candidate for catalysis in numerous organic reactions. [17-23] One of the most interesting features of metal complexes is their inherent flexibility which brings about the formation of a variety of structures. This property has gathered the attention of part of the modern scientific community to employ them in designing various functional materials. [24] Their implementation in the field of developing magnetic materials [25,26], sensors [27] and switches [28], energy storage [29,30], gas storage [31], luminescent materials for optoelectronics [32], solar cells [33], electronic devices [34], semiconductors [35] and light-emitting materials [36]

## **PREFACE**

In 2019, I embarked on my research journey for my doctoral thesis titled "**Exploration of the Chelation Property of few newly designed (N,O)-type Schiff base ligands with d-block metals and Bio-oxidase activities of their synthetic Coordination Compounds**" under the guidance of Prof. Bhaskar Biswas in the Department of Chemistry, University of North Bengal. I officially registered for my Ph.D. at the University of North Bengal, India on 01.01.2020, vide letter no. Ph.D/Cem. (1348)/532/R-2021, dated 21.04.2021.

The doctoral thesis deals with Schiff base-metal complexes and novel d-f hybrid metal complex salts that possess diverse physico-chemical properties that find applications in various research fields ranging from smart electronics to efficient catalysts to metallo-therapeutics. The objective of my study is to investigate a series of metal complexes developed using synthetic polydentate ligands, as well as commercially available ligands, in order to highlight their structural, photo-physical, spectroscopic, and bio-functional characteristics. The compounds have been thoroughly characterized using a range of spectroscopic and analytical methods, as well as single crystal X-ray diffraction studies. Furthermore, the structural features and catalytic mechanisms have been analyzed through theoretical calculations using Density Functional Theory (DFT).

Finally, the potential scientific and industrial significance of this research has been outlined, along with the future prospects of the present investigation.

## **Acknowledgement**

I would like to express my deepest gratitude to God as my utmost priority. His boundless love, mercy, and grace have been invaluable in overcoming the difficulties encountered while working on this thesis.

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I extend my heartfelt appreciation to Prof. Biswajit Sinha, Head of the department, University of North Bengal for offering the essential guidance, resources, and administrative assistance to conduct my research.

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I am grateful to our esteemed collaborators for their invaluable experimental and theoretical support, which has greatly aided me in conducting my Ph.D. research.

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I owe a great debt of gratitude to my family for their love, support, and constant motivation which have been the driving force behind my perseverance. I extend my sincere gratitude to all those who have contributed, regardless of the magnitude of their role, to this journey, with special mention to Twinkle Das and Gayetri Sarkar.

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INDIA

## LIST OF TABLES

<b>Table</b>	<b>Page No.</b>
<b>Table II.1</b> Crystallographic refinement parameters of <b>1</b> .....	40
<b>Table II.2</b> Bond angle and Bond distances of <b>1</b> .....	41
<b>Table II.3</b> Geometrical parameters of C/O–H···O hydrogen bonds (Å,°) involved in the formation of dimeric molecular units in <b>1</b> .....	41
<b>Table II.4</b> Geometrical parameters of $\pi\cdots\pi$ interactions for <b>1</b> .....	41
<b>Table II.5</b> Percentage surface area interaction of <b>1</b> .....	43
<b>Table II.6</b> Comparison of $k_{\text{cat}}$ ( $\text{h}^{-1}$ ) values for catalytic oxidation of 2-AP by reported copper(II) compounds and <b>1</b> .....	47
<b>Table III.1</b> Elemental analysis of <b>HL</b> <sup>2</sup> .....	54
<b>Table III.2</b> Elemental analysis of <b>2</b> .....	55
<b>Table III.3</b> Crystallographic data and structure refinement parameters of <b>2</b> .....	64
<b>Table III.4</b> Bond angles and bond distances value of <b>2</b> .....	65
<b>Table III.5</b> Comparison of $k_{\text{cat}}$ ( $\text{h}^{-1}$ ) values for catalytic oxidation of 2-AP by reported copper(II) compounds and <b>2</b> .....	65
<b>Table III.6</b> Percentage surface area interaction of <b>2</b> .....	67
<b>Table III.7</b> Antibacterial activity of <b>2</b> and standard drug against clinical <i>Staphylococcus aureus</i> , <i>Enterococcus</i> , and <i>Klebsiella pneumoniae</i> .....	75
<b>Table III.8</b> Target MICs $\mu\text{g}/\text{mL}$ for clinical pathogenic microorganisms.....	76
<b>Table IV.1</b> Elemental analysis of <b>HL</b> <sup>2</sup> .....	83
<b>Table IV.2</b> Elemental analysis of <b>3</b> .....	83
<b>Table IV.3</b> Crystallographic data and structure refinement parameters of <b>3</b> .....	92
<b>Table IV.4</b> Bond angles and bond distances value of <b>3</b> .....	93
<b>Table IV.5</b> Percentage surface area interaction of <b>3</b> .....	95
<b>Table IV.6</b> Hydrogen bond parameters for <b>3</b> .....	97
<b>Table IV.7</b> Comparison of $K_M$ values for catalytic oxidation of 4-MC in natural sources and by complex <b>3</b> .....	101
<b>Table IV.8</b> Redox potential data.....	103

<b>Table IV.9</b> Antibacterial activity of complex <b>3</b> and standard drug against clinical <i>Bacillus sp</i> , <i>Enterococcus</i> , and <i>E.coli</i> .....	106
<b>Table IV.10</b> Target MICs $\mu\text{g/mL}$ for clinical pathogenic microorganisms.....	106
<b>Table V.1</b> Elemental analysis of <b>H<sub>2</sub>L<sup>1</sup></b> .....	116
<b>Table V.2</b> Elemental analysis of <b>4</b> .....	116
<b>Table V.3</b> Crystallographic data and refinement parameters of <b>4</b> .....	122
<b>Table V.4</b> Bond angles and bond distances value of <b>4</b> .....	123
<b>Table V.5</b> Optimisation of complex <b>4</b> -catalyzed hydroboration of ketones.....	124
<b>Table V.6</b> Substrate scope of complex <b>4</b> -catalyzed hydroboration of ketones.....	126
<b>Table V.7</b> Substrate scope of complex <b>4</b> -catalyzed reductive amination of aldehydes with primary amines.....	169
<b>Table V.8</b> Substrate scope of complex <b>4</b> -catalyzed reductive amination of aldehydes with primary amines.....	193
<b>Table VI.1</b> Elemental analysis of <b>5</b> .....	241
<b>Table VI.2</b> Elemental analysis of <b>6</b> .....	241
<b>Table VI.3</b> Elemental analysis of <b>7</b> .....	242
<b>Table VI.4</b> Elemental analysis of <b>8</b> .....	242
<b>Table VI.5</b> EPR parameter of copper(II) complexes in different geometries.....	252
<b>Table VI.6</b> Crystallographic data and structure refinement parameters of complex <b>5</b> , <b>6</b> , <b>7</b> , <b>8</b> .....	255
<b>Table VI.7</b> Selected bond distances and angles of the complex salt <b>5</b> .....	256-257
<b>Table VI.8</b> Geometrical parameters of C–H $\cdots$ O hydrogen bonds in complex salt <b>5</b> .....	257-258
<b>Table VI.9</b> Selected bond distances and angles of complex salt <b>6</b> .....	258-259
<b>Table VI.10</b> Geometrical parameters of C–H $\cdots$ O hydrogen bonds in complex salt <b>6</b> .....	260
<b>Table VI.11</b> Selected bond distances and angles of the complex salt <b>7</b> .....	260
<b>Table VI.12</b> Selected bond distances and angles of the complex salt <b>8</b> .....	260-261
<b>Table VI.13</b> Schottky diode parameters.....	270
<b>Table VI.14</b> SCLC/Charge Transport Parameters.....	273

## LIST OF FIGURES

<b>Figure</b>	<b>Page No.</b>
<b>Fig. I.1</b> Different types of ligands.....	3
<b>Fig. I.2</b> Versatile applications of Schiff base metal complexes.....	6
<b>Fig I.3</b> Different isomers of bipyridine .....	21
<b>Fig I.4</b> Most probable binding motifs of bipyridine.....	21
<b>Fig I.5</b> Binding mode of phenanthroline with metals.....	21
<b>Fig. II.1</b> FT-IR spectra of <b>H<sub>2</sub>L<sup>1</sup></b> and <b>1</b> .....	35
<b>Fig. II.2</b> <sup>1</sup> H NMR spectrum of <b>H<sub>2</sub>L<sup>1</sup></b> .....	35
<b>Fig. II.3</b> UV-Vis spectra of <b>H<sub>2</sub>L<sup>1</sup></b> and <b>1</b> in MeOH.....	37
<b>Fig. II.4</b> Ellipsoidal plot of <b>1</b> .....	38
<b>Fig. II.5</b> Molecular packing of <b>1</b> in <i>ab</i> plane.....	39
<b>Fig. II.6</b> Intermolecular O···H and π···π interactions mediated dimer formation of <b>1</b> in crystalline phase.....	39
<b>Fig. II.7</b> Formation of 1D zigzag chain through purely π···π interactions in the growth of <b>1</b> in <i>ac</i> plane.....	39
<b>Fig. II.8</b> The Hirshfeld surfaces of <b>1</b> mapped over <i>d</i> <sub>norm</sub> , shape index and curvedness.....	42
<b>Fig. II.9</b> Fingerprint plot of <b>1</b> .....	42
<b>Fig. II.10</b> Monitoring of growth of aminophenoxazinone species upon addition of <b>1</b> to 2-AP in MeOH.....	44
<b>Fig. II.11</b> Plot of rate vs. [2-AP] in the presence of <b>1</b> in MeOH.....	45
<b>Fig. II.12</b> ESI mass spectrum of the reaction mixture between <b>1</b> and 2-AP in MeOH.....	47
<b>Fig. III.1</b> FT-IR spectra of <b>HL<sup>2</sup></b> and <b>2</b> .....	60
<b>Fig. III.2</b> UV-Vis spectra of <b>HL<sup>2</sup></b> and <b>2</b> in MeCN.....	61
<b>Fig. III.3</b> <sup>1</sup> H NMR spectra of <b>HL<sup>2</sup></b> .....	62
<b>Fig. III.4</b> <sup>13</sup> C NMR spectra of <b>HL<sup>2</sup></b> .....	62
<b>Fig. III.5</b> X-ray structure of <b>2</b> .....	63
<b>Fig. III.6</b> Hirshfeld surface of <b>2</b> .....	66
<b>Fig. III.7</b> Fingerprint plot of <b>2</b> .....	67
<b>Fig. III.8</b> Development of new electronic band upon addition of <b>2</b> to 2-AP in MeOH.....	69

<b>Fig. III.9</b> Plot of rate vs [2-AP] for the complex <b>2</b> mediated catalytic oxidation of 2-AP...	70
<b>Fig. III.10</b> Cyclic voltammogram of <b>2</b> in the presence and absence of 2-AP.....	71
<b>Fig. III.11</b> EPR spectra of <b>2</b> in the presence of 2-AP in MeCN solution.....	72
<b>Fig. III.12</b> ESI-mass spectrum of <b>2</b> in the presence of 2-AP in MeCN medium.....	74
<b>Fig. III.13</b> Electron microscope scans showing morphological changes in pathogenic bacteria.....	75
<b>Fig. IV.1</b> FT-IR spectra of <b>HL<sup>2</sup></b> and <b>3</b> .....	88
<b>Fig. IV.2</b> UV-Vis spectra of the Schiff base <b>HL<sup>2</sup></b> and <b>3</b> in MeCN medium.....	89
<b>Fig. IV.3</b> <sup>1</sup> H NMR spectrum of <b>3</b> .....	90
<b>Fig. IV.4</b> <sup>13</sup> C NMR spectrum <b>3</b> .....	90
<b>Fig. IV.5</b> X-ray structure of <b>3</b> .....	91
<b>Fig. IV.6</b> Hirshfeld surface of <b>3</b> .....	94
<b>Fig. IV.7</b> Fingerprint plot <b>3</b> .....	94
<b>Fig. IV.8</b> H···Cl interactions-based construction of 3D architecture of <b>3</b> .....	96
<b>Fig. IV.9</b> Construction of 3D architecture of <b>3</b> employing C–H···Cl and $\pi\cdots\pi$ interactions.....	97
<b>Fig. IV.10</b> Rise of new electronic band after treatment of complex <b>3</b> to 4-MC.....	100
<b>Fig. IV.11</b> Plot of rate vs [4-MeCat] for complex <b>3</b> catalyzed oxidation of 4-MC.....	100
<b>Fig. IV.12</b> Cyclic voltammogram of complex <b>3</b> in presence and absence of 4-MC.....	103
<b>Fig. IV.13</b> EPR spectrum of 4-MC in the presence of <b>3</b> .....	103
<b>Fig. IV.14</b> Electron microscope scans showing morphological changes in pathogenic bacteria.....	107
<b>Fig. IV.15</b> EDX analysis.....	107
<b>Fig. V.1</b> FT-IR spectra of <b>H<sub>2</sub>L<sup>1</sup></b> and <b>4</b> .....	118
<b>Fig. V.2</b> UV-Vis spectra of <b>H<sub>2</sub>L<sup>1</sup></b> and <b>4</b> .....	119
<b>Fig. V.3</b> <sup>1</sup> H NMR spectrum of <b>4</b> .....	120
<b>Fig. V.4</b> <sup>13</sup> C NMR spectrum of <b>4</b> .....	120
<b>Fig. V.5</b> Molecular structure of complex <b>4</b> in the solid-state.....	121
<b>Fig. V.6-Fig. V.68</b> <sup>1</sup> H NMR, <sup>11</sup> B NMR, <sup>13</sup> C NMR spectrum of 2a-4d.....	127-168
<b>Fig. V.69-Fig. V.101</b> <sup>1</sup> H NMR, <sup>11</sup> B NMR, and <sup>13</sup> C NMR spectrum of 5a-5k.....	170-191

<b>Fig. V.102-Fig. V.121</b> $^1\text{H}$ NMR, and $^{13}\text{C}$ NMR spectrum of 6a-6j.....	194-208
<b>Fig. V.122</b> Model reaction for hydroboration of a carbonyl compound using catalyst <b>4</b> ....	210
<b>Fig. V.123</b> Computational study for the formation of Pd(II)-hydride complex in the presence of HBpin.....	211
<b>Fig. V.124</b> Computational study on <b>4</b> -catalyzed hydroboration of a carbonyl compound.....	212
<b>Fig. V.125</b> Dual role of HBpin in <b>4</b> -catalyzed hydroboration of carbonyl compounds.....	212
<b>Fig. VI.1</b> FT-IR spectra for the single crystals of the complex salt <b>5</b> and <b>6</b> .....	245
<b>Fig. VI.2</b> FT-IR spectra for the single crystals of the complex salt <b>7</b> and <b>8</b> .....	246
<b>Fig. VI.3</b> UV-Vis spectra of the complex salt <b>5</b> and <b>6</b> .....	247
<b>Fig. VI.4</b> UV-Vis spectra of the complex salt <b>7</b> and <b>8</b> .....	248
<b>Fig. VI.5</b> Cyclic voltammogram of the complex salt <b>5</b> .....	249
<b>Fig. VI.6</b> Cyclic voltammogram of the complex salt <b>6</b> .....	250
<b>Fig. VI.7</b> EPR spectrum of Cu(II)-Ce(IV) complex salt <b>5</b> .....	251
<b>Fig. VI.8</b> EPR spectra of complex salt <b>6</b> .....	251
<b>Fig. VI.9</b> FE-SEM micrographs of the Cu(II)-Ce(IV) complex salt <b>5</b> .....	253
<b>Fig. VI.10</b> FE-SEM micrographs of Cu(II)-Ce(IV)-phen complex salt <b>6</b> .....	253
<b>Fig. VI.11</b> Crystal structure description of the complex salt <b>5</b> .....	261
<b>Fig. VI.12</b> Extended crystal structure description of crystal system <b>5</b> .....	262
<b>Fig. VI.13</b> Crystal structure description of crystal system <b>6</b> .....	264
<b>Fig. VI.14</b> Molecular overlay diagram of cationic units of isostructural complexes <b>6</b> and <b>8</b> .....	265
<b>Fig. VI.15</b> Crystal structure description of crystal system <b>8</b> .....	265
<b>Fig. VI.16</b> Crystal structure description of the complex salt <b>6</b> .....	266
<b>Fig. VI.17</b> Crystal structure description of crystal system <b>7</b> .....	267
<b>Figure VI.18</b> Current-voltage characteristics plot for Device A, B, C, and D.....	269
<b>Fig. VI.19</b> $dV/d(\ln J)$ vs. $J$ and $H(J)$ vs. $J$ curve for complex salts <b>5</b> , <b>6</b> , <b>7</b> , and <b>8</b> .....	269
<b>Fig. VI.20</b> Logarithmic plot of I-V characteristics curve for Device-A, B, C, and D and Capacitance vs frequency plot for complex salts <b>5</b> , <b>6</b> , <b>7</b> and <b>8</b> .....	271
<b>Fig. VI.21</b> $I$ vs. $V^2$ plot of SCLC region.....	272

## LIST OF APPENDICES

<u>Appendix</u>	<u>Page No.</u>
I: List of Publications.....	283-284
II: Seminar, Symposium Attended.....	285

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