Bull. Chem. Soc. Ethiop. **2024**, 38(5), 1337-1350.
ISSN 1011-3924
Printed in Ethiopia
Online ISSN 1726-801X
DOI: https://dx.doi.org/10.4314/bcse.v38i5.12

# SYNTHESIS AND CHARACTERIZATION OF SOME TRANSITION METAL COMPLEXES WITH SCHIFF BASE DERIVED FROM 2,6-DIAMINOPYRIDINE

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(Received May 2, 2024; Revised May 29, 2024; Accepted May 30, 2024)

**ABSTRACT**. Schiff base labeled as $H_2L_1$ was synthesized, which was derived from pyridine-2,6-diamine and 2-hydroxynaphthaldehyde. Types of complexes $[ML]Cl_2$ and $[ML(py)_2]Cl_2$, were formed with $Co^{2+}$, $Ni^{2+}$, $Cu^{2+}$, and $Zn^{2+}$. Additionally, adduct complexes $[ML(py)_2]$ were prepared in a ratio of 2:1. Diverse analytical techniques, elemental analyses, (FT-IR, UV-Vis, $^1H$ NMR), conductance measurements, and magnetic susceptibility, were employed to characterize these complexes and adducts. The data acquired validated that the ligands donor atoms act as (ONNO) tetra-dentate bibasic chelating ligands with metal ions. Depending on spectral and magnetic measurements, the suggested shapes of these complexes were reported to be either tetrahedral/octahedral in geometry. Density functional theory (DFT) was used to get some theoretical data about the generated complexes. The data obtained includes the energy of the highest and lowest occupied molecular orbitals (HOMO and LUMO), electron density, ionization potential (IP), electron affinity (EA), electronegativity (En), electrophilicity ($\dot{\omega}$), chemical hardness ($\eta$), and dipole moment ($\mu$). Different characteristics of the complexes have been investigated and explained based on these studied parameters. The molecular docking of target microorganisms of these complexes will be studied. The interaction of DNA gyrase 4ckk with the compounds visualized by LigPlot software.

**KEY WORDS**: 2,6-Diaminopyridine, 2-Hydroxynaphthaldehyde, Metal complexes, Spectral studies

## INTRODUCTION

The existence of the C=N bond within Schiff bases renders them exceptionally efficient chelating agents, particularly when a functional group such as -OH or -SH is situated near the C=N group. This arrangement allows for the formation of a 5- or 6-membered ring with the metal ion, enhancing their chelation capabilities. Considering the versatility of Schiff bases as ligands in both biological and analytical contexts, as well as their potential commercial applications, further research in this field is highly desirable [1, 2].

In coordination chemistry, the role of the Schiff laws is well known, facilitating, formation of stable complexes with transition metals. These complexes find extensive applications across various fields, including coordination chemistry itself, analytical chemistry, pigments and dyes, and the polymer industry. They are also employed in vitamins and enzymes as model biomolecules and exhibit biological and catalytic effects [3, 4].

One intriguing property of aromatic Schiff bases featuring an ortho-OH group is their ability to undergo reversible color changes when exposed to irradiation either changes in light (photochromism) or temperature (thermochromism). These optical characteristics have gained significant attention, especially given recent advancements in optical technology. Some of these Schiff bases also show potential for stimulating polymer formation [5].

Due to the keen interest in creating novel Schiff base complexes with potential applications in pharmacology and as luminescence probes, the authors synthesized and investigated complexes using Schiff bases for this work. These particular Schiff bases were produced from the reaction of pyridine 2,6-diamine, 2-hydroxy-1-naphthalene and the article shares the outcomes of their research findings.

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## EXPERIMENTAL

### *Materials*

All chemicals utilized, were of analytical quality, whether from Fluka or BDH Chemical Companies. Metal chloride [$MnCl_2.4H_2O$], or metal acetate like [$Co(CH_3COO)_2.6H_2O$], [$Ni(CH_3COO)_2.6H_2O$], [$Cu(CH_3COO)_2.2H_2O$], and [$Zn(CH_3COO)_2$], 2,6-diaminopyridine and 2-hydroxynaphthaldehyde were supplied by Sigma Aldrich company. Ethanol and dimethyl formamide (DMF) were provided by Fluka Company.

### *Instrumentation*

On spectrophotometer BRUKER (400–4000 $cm^{-1}$), infrared spectra were captured. Conductivity tests were carried out on complexes solutions at $10^{-3}$ M in DMSO at 25 °C. A JENWAY Model PCM3 conductivity meter was used for this purpose. Additionally electronic spectra at 200-1000 nm were acquired in DMSO solution ($10^{-3}$ M) using 1 cm quartz cell. This spectral measurement was performed using a SPECTRO UV-Vis AUTO instrument, operating at 110 volts and 60 hertz. An AA-7000-UN.BG.IBN-H.C.S. L atomic absorption apparatus was employed to determine the metal percentage (%). Elemental analysis was carried out (on the Euro EAE Elemental Analyzer Euro EA 3000 Italy). $^1$H-NMR spectra were acquired using TMS as a reference and DMSO-$d_6$ as internal standard and solvent in Manual Version 1.0, respectively.

### *Preparation of ligands*

Synthesis of $H_2L$ ligand adopted previously documented procedure. 2,6-Diaminopyridine (4 mmol, 0.436 g) were slowly introduced into a 10 mL alcoholic solution containing 2-hydroxynaphthaldehyde (8 mmol, 0.979 g). Next, the combination was heated to its boiling point at 60 ºC and maintained at that temperature while being stirred' for' a period of' 3 hours. The precipitate formed'was allowed to cool, washed with methanol. Brown residue subsequently subjected to further purification through column chromatography, utilizing a solvent mixture consisting of 20% ethyl acetate and 80% petroleum ether (60-90 ºC). This purification process yielded the pure product with a 68% yield and a melting point of 320 ºC [6] (Figure 1).

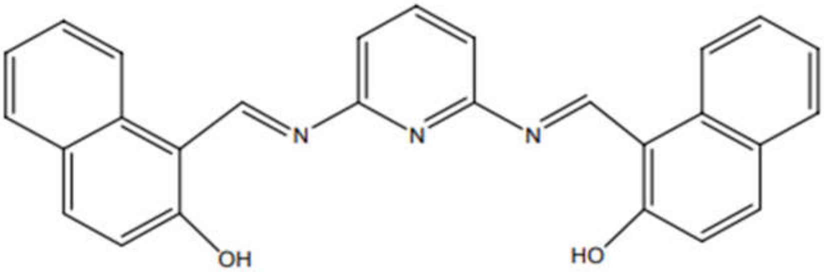


Figure 1. The structural of ligand 2,2-(1e-e)-pyridine-2,6-diylbis (azan-1-yl-1-yllidene) bis (methan-1-yl-ylidene) dinapthalede-1-ol($H_2L$).

### *Preparation of the complexes*

The ligand $H_2L$ (0.01 mol., 0.417 g) was dissolved in methanol (30 mL). Metal chloride (0.01 mol) including $MnCl_2.4H_2O$ (0.472 g) or $Co(CH_3COO)_2.6H_2O$ (0.475 g), $Ni(CH_3COO)_2.6H_2O$ (0.475 g), $Cu(CH_3COO)_2.2H_2O$ (0.480 g), and $Zn(CH_3COO)_2$, respectively, were added drop by drop over 10-15 min to the $H_2L$ ligand solution in methanol (20 mL), while continuously stirring with triethyl amine (0.001 mol, 0.101 g) dissolved in methanol (5 mL). The mixture' was' subsequently refluxed for six hours. After cooling, the' precipitate' that formed was' isolated through filtration, subjected to a cold methanol wash, and subsequently dried under vacuum pressure.

*Preparation base adduct complexes*

To create these complexes, pyridine (0.02 mol, 1.58 g) was introduced to the previously prepared complexes (0.01 mol) in a solution of methanol (50 mL), while maintaining continuous stirring and refluxing for a duration of 8 hours, or until the precipitation process was finished, on cooling, coloured solids were precipitated out, filtered, washed with cold ethanol and then dried over vacuum [7].

Table 1. The physical properties of the prepared [$H_2L$], complexes.

| Complex No. | Empirical formula | Color | m.p. (ºC) | Yield (%) | $\Lambda_M$ ($\Omega^{-1}cm^2mol^{-1}$) |
|---|---|---|---|---|---|
| | $LH_2$ | Dark yellow | 320 | 81 | |
| **1** | $[MnLH_2]Cl_2$ | Red | 310 | 79 | 170 |
| **2** | [CoL] | Reddish | 300 | 86 | 12 |
| **3** | [NiL] | Dark orang | 280 | 82 | 15.3 |
| **4** | [CuL] | Brown | 315 | 81 | 17.6 |
| **5** | [ZnL] | Pale yellow | 322 | 68 | 29 |
| **6** | $[MnLH_2(Py)_2]Cl_2$ | Dark red | 319 | 61 | 160 |
| **7** | $[CoL(Py)_2]$ | Pale Brown | 300 | 72 | 23 |
| **8** | $[NiL(Py)_2]$ | Greenish yellow | 300>d* | 69 | 18 |
| **9** | $[CuL(Py)_2]$ | Dark green | 300>d | 75 | 9.84 (8.99) |
| **10** | $[ZnL(Py)_2]$ | Orange | 300>d | 63 | 10.12 (9.86) |

*d = decomposed.

## RESULTS AND DISCUTION

Spectroscopies, FT-IR'and $^1$H-NMR'were'used to analyse the prepared ligand $LH_2$ and complexes. One can find comprehensive results in Table 2. The analytical data provided in Tables 1 and 2 indicate that these reactions involved the interaction between metal(II) acetate and manganese(II) chloride with presence of tri ethyl amine alongside the ligand. The reactions as following:

$$M(CH_3COO)_2.4H_2O + H_2L + Et_3N \rightarrow [M(L)] + Et_3N\ CH_3COO + 4H_2O \quad (1)$$

$$MnCl_2.4H_2O + H_2L + 2Et_3N \rightarrow [Mn(LH_2)]Cl_2 + 2Et_3NH + 4H_2O \quad (2)$$

$$[M(L)] \text{ or } [Mn(LH_2)]Cl_2 + 2py \rightarrow [M(L)(py)_2] \text{ or } Mn(LH_2)(py)_2]Cl_2 \quad (3)$$

$M = Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}$

Each compound is insensitive to oxygen and moisture in the air and displays consistent temperature stability. All organic solvents have been shown to be insoluble for them, with the exception of dimethyl form amide (DMF) and dimethylsulfoxide (DMSO).

Elemental analyses (C.H.N.) results indicate molar ratio (1:1) for [M:L] complexes and (1:1:2) [M:L:Py] for $[ML(Py)_2]$ complexes. The suggested formulas for the complex structures were supported by elemental analysis, which also demonstrated good agreement between the experimental and theoretical values of CHN (%) and metal content (%). The analytical data for complexes and LH$_2$ are shown in Table 2.

Table 2. Elemental analyses of LH$_2$ and its complexes.

| Complex No. | Empirical formula | Molecular weight g/mol | Elemental analysis calculated/(found) | | | |
|---|---|---|---|---|---|---|
| | | | C% | H% | N% | M% |
| | $LH_2$ | 417.27 | 77.64(77.01) | 4.55(4.30) | 10.06 (9,83) | -- |
| **1** | $[MnLH_2]Cl_2$ | 541.21 | 59.86 (58.57) | 3.51 (3.05) | 7.76 (7.20) | 10.15(10.02) |
| **2** | [CoL] | 474.20 | 68.35 (67.78) | 3.58(3.22) | 8.85 (8.14) | 12.42 (11.95) |
| **3** | [NiL] | 473.96 | 68.36 (67.98) | 3.58 (3.19) | 8.86(7.90) | 12.38 (12.11) |
| **4** | [CuL] | 478.82 | 67.66 (66.23) | 3.55 (3.08) | 8.77(8.47) | 13.27 (12.79) |
| **5** | [ZnL] | 480.66 | 67.94(66.58) | 3.92(3.02) | 8.71(8.71) | 13.60 (12.98) |
| **6** | $[MnLH_2(Py)_2]Cl_2$ | 701.21 | 63.31 (62.98) | 4.13 (3.88) | 9.98 (9.49) | 7.83 (7.44) |
| **7** | $[CoL(Py)_2]$ | 632.2 | 70. 23(69.95) | 4.27 (4.0I) | 11.07 (10.73) | 9. 32(8.89) |
| **8** | $[NiL(Py)_2]$ | 631.96 | 70.25 (69.82) | 4.27 (3.91) | 11.07 (10.89) | 9.28 (8.85) |
| **9** | $[CuL(Py)_2]$ | 636.82 | 69.72 (69.50) | 4.23 (3.92) | 10.99(10.78) | 9.97 (9.69) |
| **10** | $[ZnL(Py)_2]$ | 638.66 | 69.52 (69.41) | 4.22 (3.78) | 10.96 (10.52) | 10.23 (9.98) |

The electrical conductivity in ($10^{-3}$ M) DMSO solution for compounds typically ranging from 12 to 29 ohm$^{-1}$cm$^2$mol$^{-1}$) confirmed non-electrolytic nature of’ the complexes. However, complex (**1**, **6**) [8] stands out as an exception, as it behaves as an electrolyte, and it is a 1:2 complex (M:L) or an adduct in the case of complex [9] (Table 1).

### *FT-IR spectra*

The study and assignment of the IR spectra for the unbound ligands were carried out by carefully comparing them to the complex spectra, as detailed (Table 3), at 3400 cm$^{-1}$ a notable peak has been observed, which’ was; identified as originating from the phenolic hydroxyl group in H$_2$L. The absence of this specific peak in complex spectra suggests that phenolic oxygen of ligand coordinated with metal ions after deprotonating in all complexes [10], except for the Mn$^{2+}$ complex **1**, **6**, where the OH band remained in the same location. This indicates that there was no displacement of the hydroxyl proton in this specific complex [11].

Table 3. Infrared spectral data (wave number ν) cm$^{-1}$ of the ligand [H$_2$L] and its metal(II) compounds.

| Complex No. | νC=N | νC-O | νO-H | νM-N | νM-O |
|---|---|---|---|---|---|
| **L** | 1620 | 1270 | 3400 | -- | -- |
| **1** | 1595 | 1276 | 3405 | 540 | 590 |
| **2** | 1590 | 1278 | -- | 545 | 685 |
| **3** | 1594 | 1273 | -- | 510 | 645 |
| **4** | 1590 | 1278 | -- | 540 | 640 |
| **5** | 1590 | 1275 | -- | 525 | 595 |
| **6** | 1594 | 1272 | 3402 | 530 | 620 |
| **7** | 1484 | 1272 | -- | 540 | 790 |
| **8** | 1500 | 1275 | -- | 535 | 785 |
| **9** | 1490 | 1272 | -- | 530 | 655 |
| **10** | 1506 | 1271 | -- | 550 | 755 |

The coordination evidence is strengthened by the observation of a decrease in frequency for the phenolic C-O band, which ranges from 1270-1278 cm$^{-1}$ in all complexes spectra. LH$_2$ spectrum show a peak at 1620 cm$^{-1}$ which has been assigned to ν(C=N), it was shifted to lower frequency, approximately 25-35 cm$^{-1}$, indicating a coordinated connection between the nitrogen atom of azomethine group and metal ion in all complexes in all complexes, suggesting that the central metal ion and the nitrogen atom of the azomethine group were coordinated. Additionally, the stretching frequency ν(C=N) of pyridine'ring' noticed at'1484-1506 cm$^{-1}$ in complexes' [**6**, **7**, **8**, **9**, **10**], implying binding of pyridine ring's nitrogen of with metal ions [12]. Additional evidence for this comes from the appearance of new bands at 510-550 and 590-795 cm$^{-1}$, which were attributed to the νM–N and νM–O stretching frequencies, respectively [13].

### *Magnetism and electronic spectra*

Here's a summary of the information provided regarding the electronic spectra, magnetic susceptibility values for prepared compounds (Table 4). (1) Electronic spectra was recorded at 200–1100 nm in DMSO solvent, ligand $H_2L$ exhibit prominent electronic absorption bands at 37313 cm$^{-1}$ due to π→π* transition of the aromatic Schiff base ligand [$H_2L$]. Additionally a band at 31545 cm$^{-1}$ which corresponds to the (n→π*) transition of the (C=N) group with in the Schiff base [$H_2L$]. These absorption peaks are noticeable in complexes, but they experience shifts, confirming ligand-metal ion coordination. Furthermore, new peaks in complex spectra, falling at 27350-36200 cm$^{-1}$, that attributed to charge-transfer bands [14]. (2) The magnetic susceptibility values for $Mn^{2+}$ complexes (**1**, **6**) are at (5.12, 5.4 B.M.) which are similar to the calculated magnetic moment 5.91 B.M. for systems with five unpaired electrons. This suggests that these complexes are in a high-spin state [15]. $Mn^{2+}$ complexes do not display d-d transition bands because of the spin and parity forbidden transitions that occur within tetrahedral and octahedral environments [16, 17]. (3) The proposed structures of the $Mn^{2+}$ complexes are inferred from various measurements, with particular reliance on metal analysis among other factors [18]. (4) Magnetic moment value of $Co^{2+}$ complex **2** is 4.25 B.M. Its electronic spectra display a peak at 15838 cm$^{-1}$, due to the $^4A_2$ (F) → $^4T_1$ (P) transition, providing evidence for a tetrahedral geometry. On the other hand, the cobalt complex **7** showed magnetic'moment value'4.29 B.M. Their electronic spectra feature peaks at 10260, 19470, and 24940 cm$^{-1}$, indicating an octahedral geometry [19, 20]. (5) Complex **3** of nickel displays magnetic moment value 3.83 B.M. at room temperature, which falls within the typical range for tetrahedral Ni(II) complexes. Its spectrum exhibits a strong absorption band, which is indicative of a tetrahedral structure .On the other hand, Ni complex **8** exhibits absorption band at 25178 cm$^{-1}$, implying octahedral geometry surrounding the nickel ions [21, 22]. (6) Cu(II) complex **4** possesses a magnetic susceptibility balance of 1.91 B.M., indicating it is a high-spin complex with paramagnetic behavior. Its electronic spectra display broad peak at 10686 and 10566 cm$^{-1}$ that are compatible with tetrahedral geometry.

Table 4. Magnetic susceptibility and electronic spectra vales of metal(II) complexes.

| | | Electronic spectrum cm$^{-1}$ | | |
|---|---|---|---|---|
| Complex No. | μeff (B.M.) | d-d | Charge transfer | Suggested structure |
| **L** | -- | -- | 38210 | -- |
| **1** | 5.40 | -- | 27350 | Tetrahedral |
| **2** | 4.25 | 15838 | -- | Tetrahedral |
| **3** | 3.83 | 13230 | -- | Tetrahedral |
| **4** | 1.90 | 10686, 10566 | -- | Tetrahedral |
| **5** | -- | -- | 36200 | Tetrahedral |
| **6** | 5.12 | 19125 | -- | Octahedral |
| **7** | 4.29 | 10260, 19470, 24940 | -- | Octahedral |
| **8** | 3.71 | -- | 25175 | Octahedral |
| **9** | 1.83 | 15570 | -- | Octahedral |
| **10** | -- | -- | 33406 | Octahedral |

In contrast [23], complex **9** exhibits absorption peak at 151570 $cm^{-1}$ due to d–d transition, strongly suggesting octahedral geometry for the copper ion in this complex [24, 25]. (7) The Zn complex **5**, characterized by a $d^{10}$ electronic configuration, is diamagnetic, indicating it lacks unpaired electrons, and it is likely to have a tetrahedral geometry. Similarly, Zn complex **10** also exhibits diamagnetic behavior, which can be attributed to the $d^{10}$ electronic configuration of the metal [18]. These findings provide valuable insights into the coordination geometries and electronic properties of the examined complexes.

### *$^1H$ NMR spectra*

$^1H$ NMR (ppm) of $H_2L$ (CDCl3); δ (phenolic OH) 15.18-15.20 (d, 2H, OH); 10.03 (s, 1H, HC=N); 8.18-8.20 (d, 2H,); 7.79-7.85 (q, 2H, Ar); 7.67-7.69 (d, 2H, Ar); 7.57-7.61 (t, 2H, Ar); 7.36-7.40 (t, 2H, Ar); 7.01-7.05 (d, 2H, Ar); 6.93-6.96 (d, 2H, Ar).

### *DFT study*

To evaluate the geometrical parameters and investigate the revival of the investigation chemicals, a computational study is being carried out. The Gauss View 5.0.8 presentation was used to draw structures. Ligands and all metal complexes shall be optimized at the level of B3LEP [26-28] using 6.311G++ as a basis. 6.311G++ is a large set of rules containing the functions of dispersed and polarized waves that should take into account.

The characteristics associated with ion species containing atoms such as Chemcraft [26] have been used to visualize the optimal compounds geometry, and to indicate that structures at the same level of theory are truly miniature, the harmonic frequencies must be calculated. Using the virtual convergence criteria provided by the software, optimization has been accomplished without imposing any restrictions on uniformity. In this work, Gausian 09 routine was used in the molecular calculations. Coordination chemicals and organic molecules works well to this computational approach. Chemical potential (μ) has been defined by conceptual DFT as the first derivative of energy with respect to the number of electrons.

$$\mu = \left(\frac{\partial E}{\partial N}\right) \boldsymbol{\vartheta}(\boldsymbol{r}) \tag{4}$$

Chemical hardness (η) is the second derivative of energy divided by 2 with respect to the electrons number at a constant external pressure, resulting in the first derivative of energy with respect to the number of electrons. Electron affinity (EA) and ionization potential (IP) have been used to calculate chemical potential (μ) and chemical hardness (n), resulting in [28]

$$\boldsymbol{\mu} = -\left(\frac{\boldsymbol{IP+EA}}{\mathbf{2}}\right) \text{ and } \boldsymbol{n} = \left(\frac{\boldsymbol{IP-EA}}{\mathbf{2}}\right) \tag{5}$$

The highest occupied molecular orbital (EHOMO) and the lowest occupied molecular orbital (ELUMO) were related to electron affinity (EA) and ionization potential (IP) according to Koopman's theorem

$$\boldsymbol{\mu} = \left(\frac{\boldsymbol{ELUMO-EHOMO}}{\mathbf{2}}\right) \boldsymbol{and} \ \boldsymbol{n} = \left(\frac{\boldsymbol{ELUMO+EHOMO}}{\mathbf{2}}\right) \tag{6}$$

Compound's electrophilic can be measured by electrophilicity as suggested by Parr and coworkers, which may be written as

$$\text{ɯ} = \frac{\mu 2}{2n} \tag{7}$$

Table 6 contains ($\mu$), ($\eta$), and electrophilicity of the ligands and complexes. Using the minimum electrophilicity principle, we may anticipate the reactivity of prepared compounds. The most stability compound must have the lowest electrophilicity, according to the minimum electrophilicity principle. HOMO and LUMO data of the ligand have been utilized in the derivation of the chemical potential ($\mu$), chemical hardness ($\eta$), and electrophilicity (Ш) and its complexes (Figure 2, Table 5). The order of reactivity for metal complexes is as follows:

Co(II) > Zn(II) > Mn(II) > Ni(II) > Cu(II) > ligand, they are more reactive than ligands [29-30].

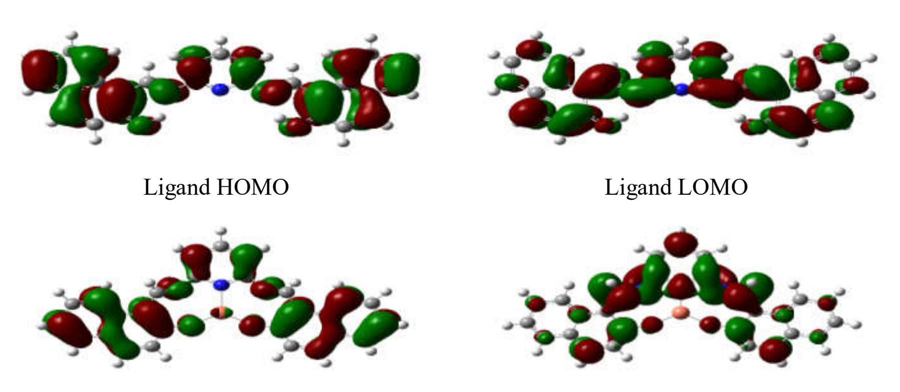
Table 5. HOMO and LOMO, ΔE (eV), $\eta$, $\mu$, and Ш of prepared compounds.

| Complexes | HOMO | LOMO | ΔE (eV) | $\eta$ | $\mu$ | Ш |
|---|---|---|---|---|---|---|
| L | -3.284 | -2.841 | 0.443 | 0.222 | -3.063 | 1.0388 |
| Mn[L] | -4.454 | -1.720 | 2.734 | 1.367 | -3.087 | 6.5134 |
| Co[L] | -8.483 | -7.968 | 0.515 | 0.258 | -8.226 | 8.7111 |
| Ni[L] | -7.827 | -7.545 | 0.282 | 0.141 | -7.686 | 4.1647 |
| Cu[L] | -9.475 | -9.348 | 0.127 | 0.064 | -9.412 | 2.8120 |
| Zn[L] | -4.931 | -2.537 | 2.394 | 1.197 | -3.740 | 8.345 |

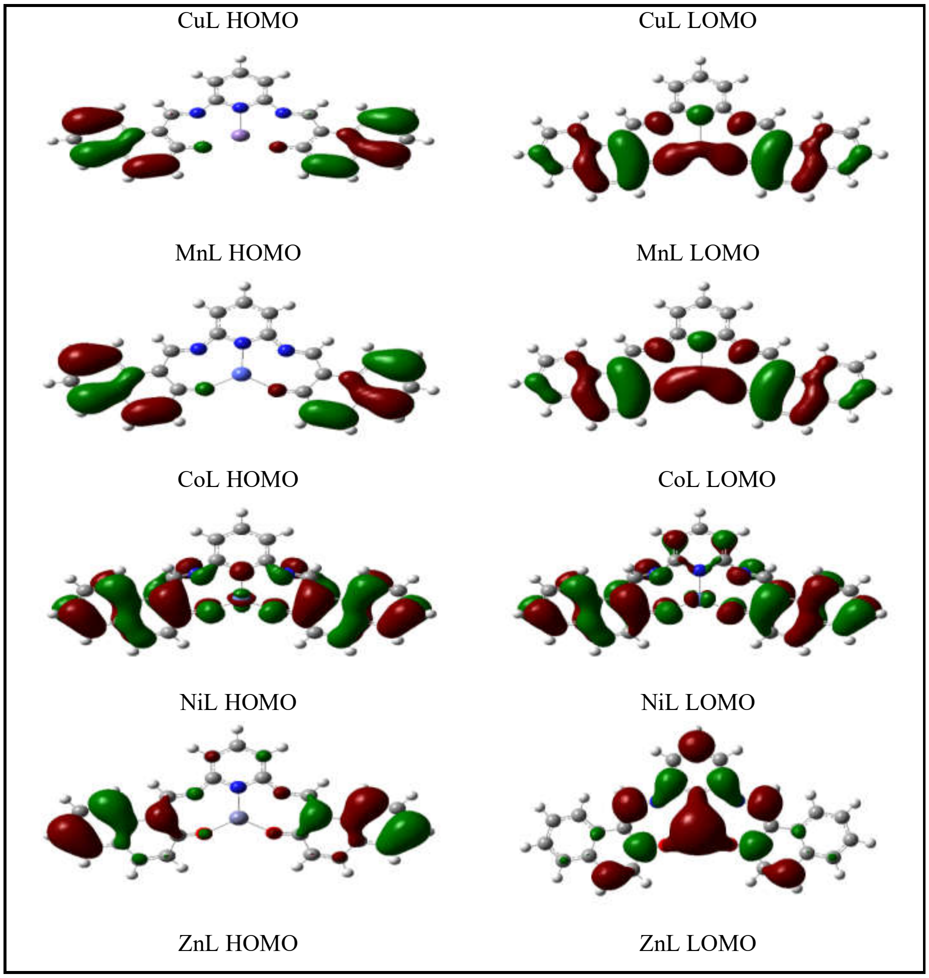
*Molecular docking studies*

DNA gyrase is a target for developing new antimicrobials due to microbial resistance to commonly used antibiotics [31]. Docking experiment was performed using the on line server CB-dock2 [32] which can be accessed via https://cadd.labshare.cn/cb-dock2/php/index.php. The enzyme target was DNA gyrase subunit A (pdb ID: 4ckk) according to method [31]. Table 6 shows the results of molecular docking and the interactions involved. Interactions were analyzed using LigPlot software [33].

The first compound was the best forming two hydrogen bonds with chain D of DNA gyrase A model followed by second compound which formed only one hydrogen bond with Asp157 amino acid. All the compounds formed hydrophobic interactions by the same amino acid residues. The study of Rahimi *et al*. [31] showed that the compound ZINC67829151 from zinc database has binding affinity of -12.6 kcal/mol by molecular docking with Auto dock 4.2 among 11830 compounds. Their study found three compounds with different chemical structures as potential lead compounds. In addition [34] used Auto dock 4.2 to dock cyclic di phenyl phosphonates against the same target with binding energies ranged between -8.65 to -5.9 kcal/mol, Figure 3.


Ligand HOMO

Ligand LOMO



CuL HOMO

CuL LOMO

MnL HOMO

MnL LOMO

CoL HOMO

CoL LOMO

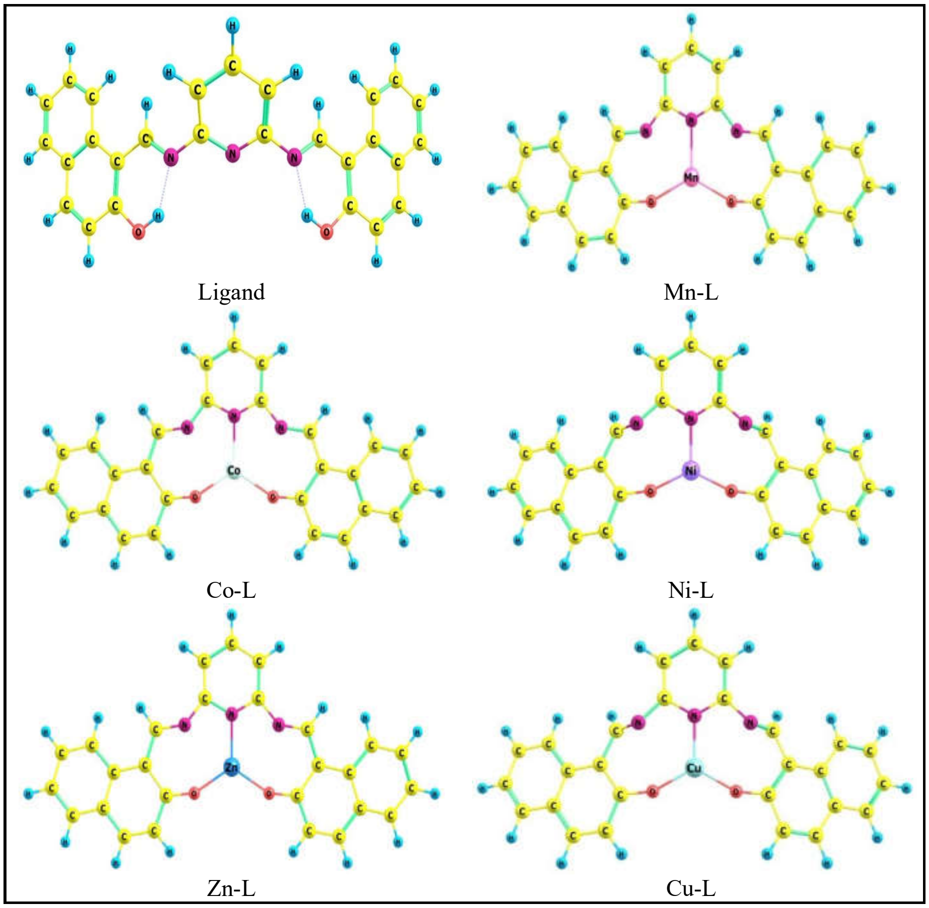
NiL HOMO

NiL LOMO

ZnL HOMO

ZnL LOMO

Figure 2. (a) HOMO and LOMO of ligand-X (X = $Mn^{+2}$, $Co^{+2}$, $Ni^{+2}$, $Cu^{+2}$, $Zn^{+2}$) complexes.



Ligand Mn-L

Co-L Ni-L

Zn-L Cu-L

Figure 2.(b) Ligand-X (X = $Mn^{+2}$, $Co^{+2}$, $Ni^{+2}$, $Cu^{+2}$, $Zn^{+2}$) complexes optimized geometry structures

Table 6. Molecular docking results of the compounds against shikimate kinase enzyme.

| Compound | Docking score (kcal/mol) | Hydrogen bonds | Hydrophobic interactions |
|---|---|---|---|
| [CuL] | -5.1 | Asp157 | Ile155, Val146, Pro156, Arg46, Arg47, Asp147 |
| $[MnLH_2]Cl_2$ | -5.1 | Asp157 | Ile155, Val146, Pro156, Arg46, Arg47, Asp147, Pro43 |
| $[CoL(Py)_2]$ | -5.1 | -- | Ile155, Val146, Pro156, Arg46, Arg47, Asp147, Pro43, Asp157 |
| $[MnLH_2(Py)_2]Cl_2$ | -5.1 | -- | Ile155, Val146, Pro156, Arg46, Arg47, Asp147, Pro43, Asp157 |

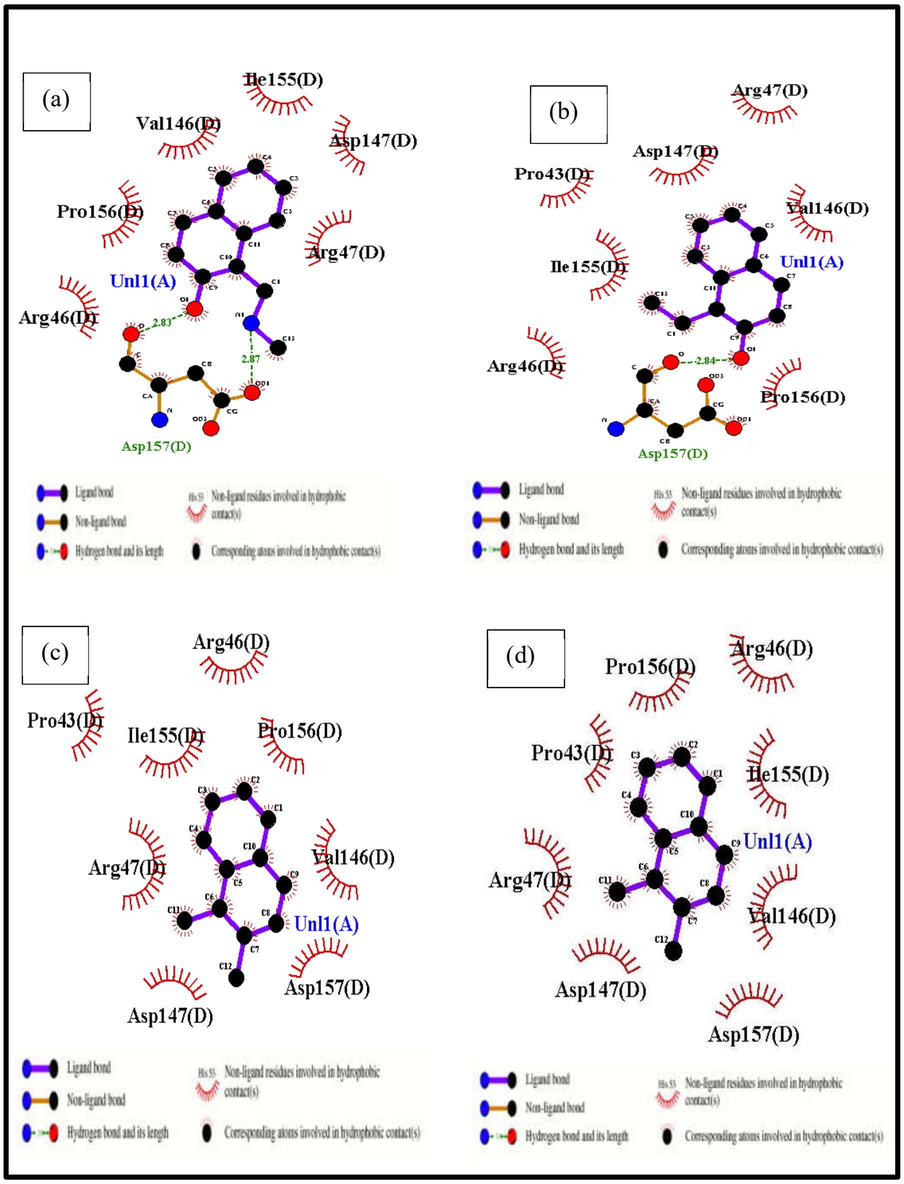
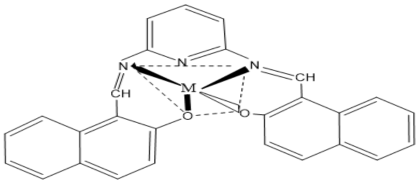
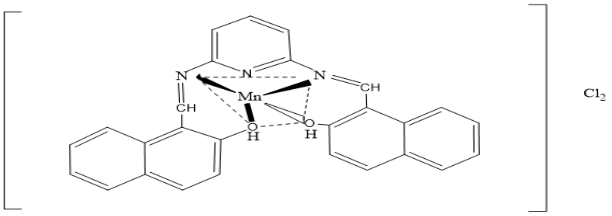
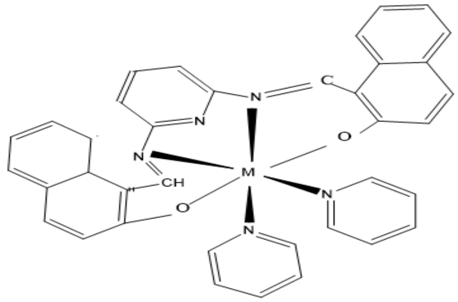


Figure 3. (a) The interaction of DNA gyrase 4ckk with the compound [CuL] visualized by LigPlot. (b) The interaction of DNA gyrase 4ckk with the compound $[MnLH_2]Cl_2$ visualized by LigPlot. (c) The interaction of DNA gyrase 4ckk with the compound $[CoL(Py)_2]$ visualized by LigPlot. (d)The interaction of DNA gyrase 4ckk with the compound $[MnLH_2(Py)_2]Cl_2$ visualized by LigPlot.



M=Co(II),Ni(II),Cu(II),Zn(II)





M= Mn(II), Co(II), Ni(II), Cu(II),Zn(II).

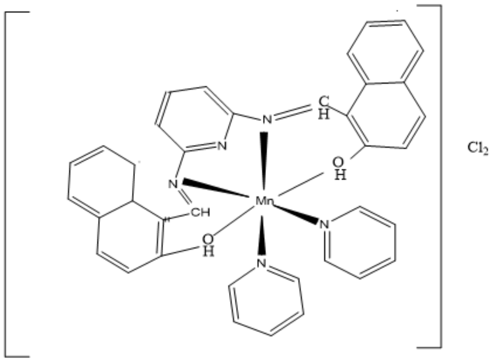


Figure 4. The proposed structures of the compounds.

## CONCLUSION

The synthesized Schiff base $H_2L$ functions as a bidentate ligand forming coordination'bonds'with metal ions'by interacting azomethine nitrogen (-C=N-) and phenolic oxygen (-OH). Coordination of metal ion to ligand was substantiated by spectral analyses. The collected data validates that the complexes are mononuclear in nature and adopt either tetrahedral or octahedral geometries. The proposed structures of the compounds can be illustrated as shown in Figure 4.

## ACKNOWLEDGMENTS

The authors thank the Deanship of the College of'Science'and the Head of'the Chemistry' Department as well as the staff of the scientific laboratories in the Chemistry Department for facilitating the task of conducting this research.

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