

Preparation, Spectroscopic Characterization and Theoretical Studies of Transition Metal Complexes with 1-[(2-(1*H*-indol-3-yl)ethylimino)methyl]naphthalene-2-ol Ligand

VIAN YAMIN JIRJEES¹, VEYAN TAHER SULEMAN¹, ABBAS ALI SALIH AL-HAMDANI^{2*} and SUZAN DURAI AHMED³

¹Department of Chemistry, College of Science, University of Dohuk, Dohuk, Iraq

²Department of Chemistry, College of Science for Women, University of Baghdad, Baghdad, Iraq

³Department of Chemistry, College of Education for Pure Science (Ibn Al-Haitham), University of Baghdad, Baghdad, Iraq

*Corresponding author: E-mail: abbas_alhamadani@yahoo.co.uk

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A new Schiff base [1-((2-(1*H*-indol-3-yl)ethylimino)methyl)naphthalene-2-ol] (HL) has been synthesized by condensing (2-hydroxy-1-naphthaldehyde) with (2-(1*H*-indol-3-yl)ethylamine). In turn, its transition metal complexes were prepared having the general formula; [Pt(IV)Cl₂(L)₂], [Re(V)Cl₂(L)₂]Cl and [Pd(L)₂], 2K[M(II)Cl₂(L)₂] where M(II) = Co, Ni, Cu] are reported. Ligand as well as metal complexes are characterized by spectroscopic techniques such as FT-IR, UV-visible, ¹³C & ¹H NMR, mass, elemental analysis. The results suggested that the ligand behaves like a bidentate ligand for all the synthesized complexes. On the other hand, theoretical studies of the ligand as well its metal complexes were conducted at gas phase using HyperChem 8.0. These metal complexes exhibited good antibacterial activity.

Keywords: Ethylamine, 2-Hydroxy-1-naphthaldehyde, Thermal analysis, Transition metal complexes, Schiff base.

INTRODUCTION

Schiff bases have been considered like versatile ligands which provide probability to the design metal complexes for helpful in biological activities. Numerous works based on bi-, tri- and tetradentate Schiff bases originated from different diamine or carbonyl compounds [1,2] are reported in the literature. These Schiff bases complexes containing O, N, S donor of chelates possess an unusual distribution. In these cases, presence of donor atoms at complexes could improve antitumor, antifungal, antibacterial activities, *etc.* [3]. Structural chemistry like symmetrical and/or unsymmetrical complexes depend upon the nature of ligands and its structural stereochemistry as well number of donor atoms also plays an important role in the enhancement of the biological activities [4]. The wide range of Schiff base complexes are applied for the organic syntheses specially in the design of medicines [5]. Moreover, they also exhibit in various biological, analytical and catalytic activities [6]. Indole based Schiff bases have extensive biological activities *viz.*, antiviral, anticancerogenic, antibacterial, antifungal and antitumor [7]. Therefore, metal complexes of Schiff bases play a

vital role at dominant gene expression, inhibition of cell division henceforth are also applied in chemotherapy, *etc.* However, the problem concerned for these complexes are the prepared separation in a solution that leads to highly reactive classes which are incapable into amount for drug aims like DNA. This reaction is rapid and the formation of highly interacting Ni(II) and Pd(II) complexes consist of bulky ligands such as triphenylphosphine [8]. In recent works, due to the presence of *d*¹⁰ electronic distribution, received a lot for interest in organic, ecological and biochemistry chemistry. With respect to 20 known metal enzymes and which transition metals are in general tetrahedral coordination also associated with solid donor atoms like nitrogen [9]. Moreover, metal complexes of Schiff bases have important applications, especially in biological area in extension to their significant roles in catalysis as well as in organic composition [7,8,10].

EXPERIMENTAL

All the chemicals and reagents have been acquired from the commercial sources (Sigma-Aldrich, Merck, *etc.*) and used without further purification.

NMR spectra have been measured at DMSO-*d*₆ solution employing Bruker AMX 400 MHz and JEOL Lambda 400 MHz spectrum. Elemental analyses (C, H and N) have been analyzed by using Perkin-Elmer automatic equipment model 240.B. Melting points have been measured on a Buchi SMP-20 poetical melting point device and are uncorrected. Metal contents have been analyzed using a Shimadzu 680 G Atomic Absorption Spectrometer. Conductivity measurements were conducted by employing DMSO solutions using a Jenway 4071 digital conductivity meter at room temperature. Chlorine has been specified employing the method of potentiometer titration by a 686-Titro processor-665Dosimat-Metrohm Swiss. IR analysis were carried out using Shimadzu FT-IR 3800 spectrophotometer having KBr or CsI discs in the range of 4000-400 cm⁻¹. Electronic spectral analysis have been carried out in DMSO at 25 °C utilizing a Shimadzu 160 Spectrophotometer. Mass spectra have been acquired through positive Electron-Influence (EI) as well Fast Atom Bombardment (FAB) has been registered at a VG auto spec micromass spectrometer.

Synthesis for ligand [1-((2-(1*H*-indol-3-yl)ethylimino)-methyl)naphthalene-2-ol (HL): 2-Hydroxy-1-naphthaldehyde (0.847 g, 0.00492 mol) dissolved in methyl alcohol solution (10 mL) has been mixed to an methanolic solution (15 mL) of 2-(1*H*-indol-3-yl)ethylamine (0.788 g, 0.00492 mol). The mixture was refluxed about 16 h with constant stirring. A dark yellow glossy solid has been generated and thereafter recrystallized the solid from diethyl ether:ethyl alcohol (1:1) solvent. The solid had been dehydrated over anhydrous CaCl₂ (**Scheme-I**). Yield: 89 %, m.p.: 247-248 °C. The ¹H NMR spectrum of Schiff base (HL) displays various peaks at δ = 7.008-8.084 ppm (m, 11H, Ar-H), which is attributed due to aromatic protons [11], peak at δ = 12.117 ppm (s, 1H, N-H) is due to the presence of proton of amine [12]. The peak at δ = 2.103 ppm is assigned to (tri, 2H, C-CH₂) group and the peak at δ = 3.024-3.426 ppm (tri, 2H, N-CH₂) [13]. ¹³C NMR (100.622 MHz, DMSO-*d*₆): δ 177.22 (C11), 163.25 (C21), 144.67 (C14,15,16,17), 139 (C20), 127 (C5, 6), 124.31 (C13,18), 109.83 (C12), 105.95 (C7), 77.25 (C10), 56.93 (C9).

Preparation of metal complexes: The Schiff base metals complexes have been synthesized through refluxing the ethanolic solution of equimolar Schiff base and corresponding metal salts at 250 mL in two necked flask for 3 h. The metal salts used in present study are chloro salts of Re(V), Pt(IV),

Pd(II), Co(II), Ni(II) and Cu(II). The solid precipitate present in the reduced volume of mother liquid has been isolated through filtration. The crude solid has been recrystallized using ethyl alcohol, dried and finally kept in vacuum desiccators.

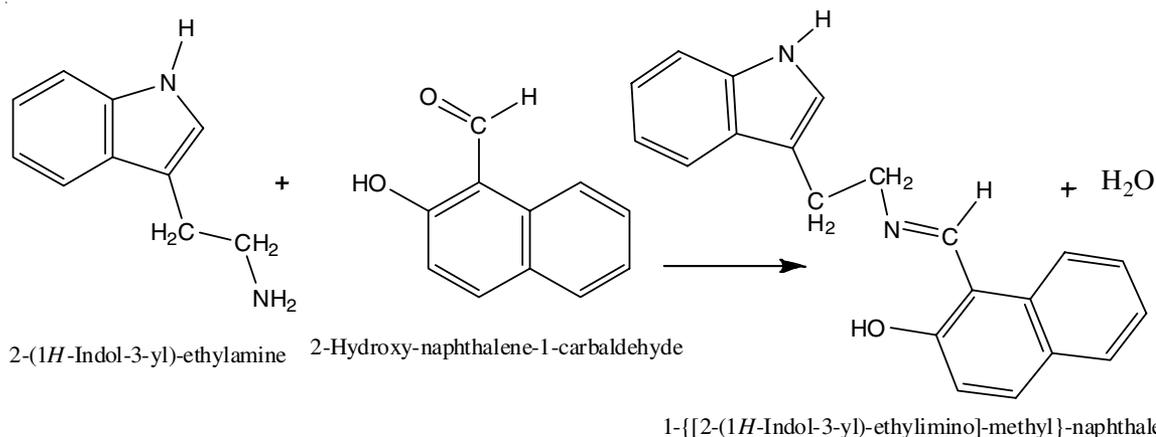
Antibacterial activity: All the synthesized metal complexes and Schiff base ligand have been examined against *S. aureus* (Gram positive) and *P. aeruginosa* (Gram negative) bacteria and fungi such as *Penicillium expansum*, *Fusarium graminearum*, *Macrophomina phaseolina* and *Candida albicans*, using the method of diffusion wall of agar by utilizing DMSO solvent. The condensation of compounds at this detection was (10⁻³ M) through employing disc sensibility check. This method includes the exposition to zone inhibition toward the diffusion from microorganism on agar plate. The plates have been brood within 24 and 48 h from bacteria and fungi, respectively at 37 °C.

Theoretical calculations: HyperChem 8.0 program is an advanced molecular mode, a powerful accounting package known owing to its quality, elasticity, easy to use, retractor 2D visualization as well as vitality for quantity chemical calculations, molecular mechanics and dynamics. In the present work, parameterization process 3 (PM3) has been applied with calculation using heat energy binding with each metal complexes. The PM3 and AMBER are more public than semi-experimental manner due to the availability for algorithms. It has parameterized primarily for organic molecules and some selected transition metals [14,15].

RESULTS AND DISCUSSION

Bidentate complexes (Fig. 1) were synthesized by the interaction between metal ions and a Schiff base at molar ratio of 1:2 (metal:ligand). Synthesized solid Schiff base ligand and complexes are highly stable in the room temperature. Ligand and metals complexes are generally soluble in hot DMF and DMSO and other physico-chemical data are given in Table-1. The analytical data are satisfactorily consistent with suggested stoichiometry for complexes. It is worthwhile to mention that ligand and metal complexes can act as dyestuffs because they exhibit high molar extinction coefficients.

Mass spectrum: Mass spectrum of ligand (HL) emphasizes the possible formula by exhibiting a peak at 314.3 *m/z*, which is identical to that of a Schiff base moiety [(C₂₁H₁₈N₂O) of atomic mass 314.38]. The chains exhibit peaks at 205, 204, 79.4, and 36 *m/z*, which may be attributed to diverse fragments.



Scheme-I: Synthesis route of the Schiff base

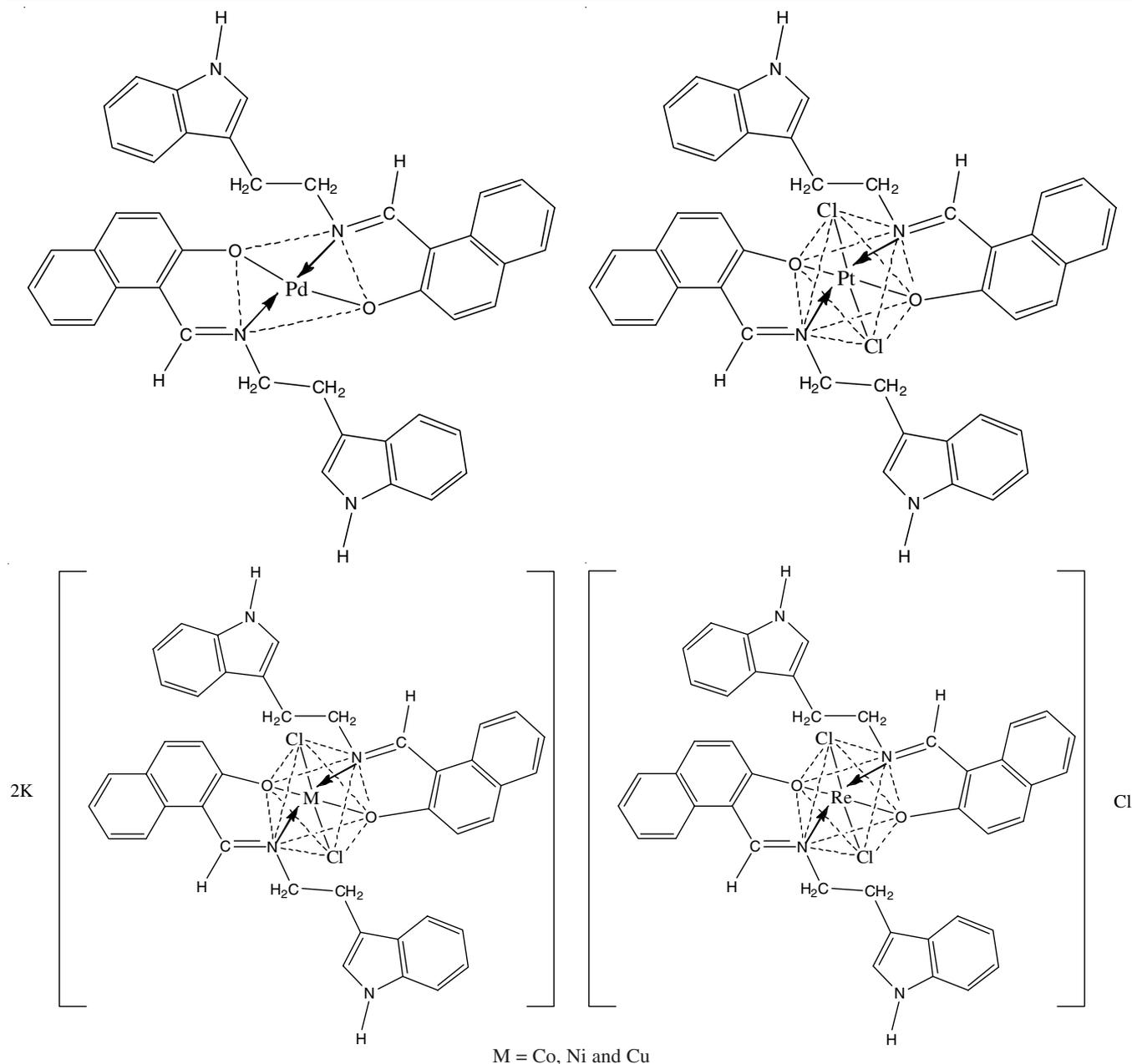


Fig. 1. Structures of the metal complexes

TABLE-1
ANALYTICAL AS WELL PHYSICAL DATA TO THE LIGAND ALSO COMPLEXES

Compounds	m.f. m.w.	Colour	m.p. (°C)	Yield (%)	Elemental microanalysis (%): Calcd. (found)				
					C	H	N	M	Cl
HL	C ₂₁ H ₁₈ N ₂ O 314.38	Dark yellow	247-248	89	80.23 (79.72)	5.77 (6.13)	8.91 (9.18)	–	–
[Pd(L) ₂]	C ₄₂ H ₃₄ N ₄ O ₂ Pd 733.17	Red brown	301 d	75	68.80 (67.91)	4.67 (5.16)	7.64 (8.07)	14.52 (13.93)	–
K ₂ [NiCl ₂ (L) ₂]	C ₄₂ H ₃₄ N ₄ O ₂ NiCl ₂ K ₂ 834.54	Dark greenish	309 d	89	60.45 (61.17)	4.11 (3.37)	6.71 (7.70)	7.03 (8.01)	8.50 (9.15)
[PtCl ₂ (L) ₂]	C ₄₂ H ₃₄ N ₄ O ₂ Cl ₂ Pt 892.73	Red brown	287	80	56.51 (55.88)	3.84 (4.14)	6.28 (7.01)	21.85 (22.16)	7.94 (7.75)
K ₂ [CoCl ₂ (L) ₂]	C ₄₂ H ₃₄ N ₄ O ₂ CoCl ₂ K ₂ 834.78	Green	327 d	76	60.43 (61.31)	4.11 (4.49)	6.71 (7.18)	7.06 (7.13)	8.49 (9.16)
K ₂ [CuCl ₂ (L) ₂]	C ₄₂ H ₃₄ N ₄ O ₂ CuCl ₂ K ₂ 839.39	Brown	270 d	70	60.10 (61.01)	4.08 (5.01)	6.67 (5.89)	7.57 (8.15)	8.45 (7.78)
[ReCl ₂ (L) ₂ Cl]	C ₄₂ H ₃₄ N ₄ O ₂ ReCl ₃ 919.31	Brown	332 d	86	54.87 (55.13)	3.73 (4.14)	6.09 (5.81)	–	11.57 (10.67)

d = decompose

Pt(IV) complex: Electronic spectrum of [PtCl₂(L)₂] confirms the possible formula because it exhibits a peak at 892 *m/z*, which confirms to a complex moiety [(C₄₂H₃₄N₄O₂Cl₂Pt)] of atomic mass 892.73. The peaks at 639 and 365 *m/z* may be attributed to diverse fragments. Electronic spectrum of [PdL₂] indicates the possible chemical formula by exhibiting a peak at 733 *m/z*, which confirms the complex moiety [(C₄₂H₃₄N₄O₂Pd)] of atomic mass 733.17. Chain with peaks at 633, 562.5, 337.5, 225, 205, and 204 *m/z* may be attributed to diverse fragments [16].

Electronic spectra and magnetic moments studies: Table-2 indicates the values of ligand absorption and intensive absorption is observed at 33090 and 39087 cm⁻¹, which may be assigned to $\pi \rightarrow \pi^*$ also $n \rightarrow \pi^*$, respectively. The value of magnetic moment 3.70 B.M. indicates that Co(II) complex has octahedral geometry [17,18]. The electronic spectrum of Co(II) complex appeared as two wide peaks at 16266.1, 14749.2 and 11001.1 cm⁻¹, which were designated as ⁴T_{1g} → ⁴T_{1g}(P) (ν₃), ⁴T_{1g} → ⁴A_{2g} (ν₂) and ⁴T_{1g} → ⁴T_{1g}(F) (ν₁) transition, respectively. Furthermore, the peak at 24937.6 cm⁻¹, designated as M → L (C.T.) and 37174.7 cm⁻¹, was assigned to a ligand field. The Ni(II) complex shows peaks at 23041, 20576 and 12722.6

cm⁻¹, which indicated ³A_{2g} → ³T_{1g}(P), ³A_{2g} → ³T_{1g}(F) and ³A_{2g} → ³T_{2g}(F) transition, respectively, and at 36363.6 cm⁻¹, which was attributed to a ligand field proposing octahedral geometry of ligands around Ni(II) ions. The value of magnetic moment (2.91 B.M.) of Ni(II) complex is consistent with octahedral geometry [13,17,18]. The Pt(IV) complex jointly with the μ_{eff} value (Table-3) shows four peaks in 24390.2, 20618.5 and 19230.7 cm⁻¹ whom specified into ¹A_{1g} → ¹T_{3g}, ¹A_{1g} → ¹T_{2g} also ¹A_{1g} → ¹T_{1g} transition, respectively as well 32786.8 cm⁻¹ assigned to M → L (C.T.) also 37174.7 cm⁻¹, assigned to ligand field, which suggested octahedral geometry of Pt(IV) complex [17,19]. In case of Pd(II) complex, bands were assigned to the ligand field, ¹A_{1g} → ¹B_{1g} and ¹A_{1g} → ¹A_{2g} (35971.2, 20283.9, and 13071.8) cm⁻¹, respectively; furthermore, this indicates square planar geometry around the Pd(II) ion, moreover, the value of magnetic moment to this complex is consistent with square planar geometry [17,20]. Electronic spectra for Cu(II) complexes showed low energy absorption bands at 20242.9 and 36363.6 cm⁻¹, which can be attributed to the transitions ²E_g → ²T_{2g} and ligand field, respectively. These bands indicate the octahedral geometry of Cu(II) ion and also the magnetic moment value of 1.66 B.M. of Cu(II) complex is also consistent with octahedral

TABLE-2
ELECTRONIC DATA, MAGNETIC MOMENTS AND MOLAR CONDUCTIVITY OF THE METAL COMPLEXES

Complexes	ABS	λ (nm)	ν (cm ⁻¹)	ε (L mol ⁻¹ cm ⁻¹)	Assignment	Ω (Ohm ⁻¹ cm ² mol ⁻¹)	μ _{eff} (B.M)	Proposed geometry
[ReCl ₂ (L) ₂]Cl	2.459	275	36363.6	2459	Ligand field + C.T.	82	2.95	Octahedral
	0.983	489	20449.8	983	³ T _{1g} → ³ A _{2g}			
	0.546	637	15698.5	546	³ T _{1g} → ³ T _{1g} (P)			
	0.208	715	13986	208	³ T _{1g} → ³ T _{2g} (F)			
[PtCl ₂ (L) ₂]	1.688	269	37174.7	16880	Ligand field	25	Diamagnetic	Octahedral
	2.109	305	32786.8	21090	C.T.			
	0.741	410	24390.2	741	¹ A _{1g} → ¹ T _{3g}			
	0.627	485	20618.5	627	¹ A _{1g} → ¹ T _{2g}			
	0.588	520	19230.7	588	¹ A _{1g} → ¹ T _{1g}			
[Pd(L) ₂]	2.414	278	35971.2	24140	Ligand field	27	Diamagnetic	Square planar
	0.605	493	20283.9	605	¹ A _{1g} → ¹ B _{1g}			
	0.101	765	13071.8	101	¹ A _{1g} → ¹ A _{2g}			
K ₂ [CuCl ₂ (L) ₂]	2.082	275	36363.6	20820	Ligand Field	145	1.66	Octahedral
	0.604	494	20242.9	604	² E _g → ² T _{2g}			
K ₂ [CoCl ₂ (L) ₂]	1.850	269	37174.7	1850	Ligand Field	159	3.70	Octahedral
	2.472	401	24937.6	401	C.T.			
	0.061	615	16266.1	615	⁴ T _{1g} → ⁴ T _{1g} (P)			
	0.106	678	14749.2	678	⁴ T _{1g} → ⁴ A _{2g} (F)			
	0.009	909	11001.1	909	⁴ T _{1g} → ³ T _{1g} (F)			
K ₂ [NiCl ₂ (L) ₂]	2.401	275	36363.6	24010	Ligand Field	166	2.91	Octahedral
	0.203	434	23041	203	³ A _{2g} → ³ T _{1g} (P)			
	0.232	486	20576	232	³ A _{2g} → ³ T _{1g} (F)			
	0.084	786	12722.6	84	³ A _{2g} → ³ T _{2g} (F)			

TABLE-3
FTIR SPECTRUM DATA (cm⁻¹) OF THE METAL COMPLEXES

Compounds	C-H aromatic aliphatic	ν(N-H)	ν(C=N)	ν(O-H)	ν(M-N)	ν(M-O)
HL	3021, 2987	3243	1694	3575	–	–
[ReCl ₂ (L) ₂]Cl	3026, 2982	3240	1666	–	534	484, 423
[PtCl ₂ (L) ₂]	3043, 2988	3237	1635	–	586, 536	491, 474
[Pd(L) ₂]	3022, 2979	3239	1676	–	530	480, 424
K ₂ [CuCl ₂ (L) ₂]	3043, 2957	3241	1634	–	582, 536	500, 474
K ₂ [CoCl ₂ (L) ₂]	3023, 2937	3240	1682	–	534	484, 423
K ₂ [NiCl ₂ (L) ₂]	3021, 2968	3236	1637	–	580, 540	490, 420

geometry [17,19]. The spectrum for Re(V) complex, (μ_{eff} 2.95) exhibits four peaks at 36363.6, 20449.8, 15698.5 and 13986 cm^{-1} , which indicated ligand field (C.T.), ${}^3T_{1g} \rightarrow {}^3A_{2g}$, ${}^3T_{1g} \rightarrow {}^3T_{1g}$ (p) and ${}^3T_{1g} \rightarrow {}^3T_{2g}$ (F) transition, respectively. Furthermore, these data indicated the octahedral geometry for Re(V) complex [17,19]. Moreover, molar conductivity of these complexes are also found consistent for electrolytes of every complex with 1:2 electrolyte and 1:1 electrolytes for Re complex but with non-electrolytes for Pt and Pd complexes.

Infrared analysis: The ligand exhibits the characteristic bands at 3575, 1307, 3243 and 1694 cm^{-1} which is attributed to $\nu(\text{OH})$ phenolic, $\nu(\text{C-O})$ phenolic, $\nu(\text{N-H})$ and $\nu(\text{C=N})$ azomethine, respectively. The IR spectra of the complexes exhibited that ligand bands shifts due to the formation of complexes (Table-3) [21,22]. Furthermore, the $\nu(\text{C=N})$ band of ligand was observed at 1694 cm^{-1} and also this band shifted to lower frequencies through (28-22 cm^{-1}) in complexes. This indicates that the ligand was coordinated to the metal ions through N-atom (azomethine) [11,13].

The results also revealed that the ligand was coordinated with metal ions by N-atom. Reduction in bond order on complexation, may be caused by delocalization of electron metal intensity (t_{2g}) into the π -system of ligand. These shifts indicate the coordination of the ligand through nitrogen from the group of azomethine into metal ions. The $\nu(\text{N-H})$ band of free ligand at 3243 cm^{-1} did not shift in the complexes. At low frequencies, the complexes exhibited bands near 582-534 cm^{-1} , which are attributed to $\nu(\text{M-N})$. Additionally, bands near 403-378 cm^{-1} were assigned to $\nu(\text{M-Cl})$ with complexes. Therefore, the Cl atom was considered coordinated with all complexes, except for palladium complex, which did not exhibit a band to the $\nu(\text{M-Cl})$ [11,23,24]. Moreover, ligand offers a wide band on approximately 3575 cm^{-1} because intramolecular H-bonded

of hydroxide group. This band vanishes at their corresponding metal complexes showing the coordination of phenol oxygen into metal ion by removing the proton [13]. Comparison of experimental results and theoretical vibration frequencies are listed in Table-4.

Theoretical study: Vibrational spectra of the ligand and complexes were calculated by using a semi-empirical (PM3) method. The distortion may occurred because the approximate harmonic oscillators lack an electron connection. Previous study [23] reported that frequencies coupled for Hartre-Fock Theory proximate a quantum harmonic oscillator rounding which tends to be 10 % high. Theoretically possible structures from metal complexes with ligand have been calculated to match the most possible pattern building steady structure. These forms display the calculated optimal geometries with ligands and its metal complexes. The results from PM3 method from calculation at gas phase for the binding energies and heat values of formation of Co(II), Ni(II), Pd(II), Re(V) and Pt(IV) complexes are listed in Table-5.

Electrostatic potential: Electron allocation decides the electrostatic potential (EP) of molecules and characterizes the interaction of energy to the molecular system for positive dot transport. Thus, it is useful in finding sites from reaction at a molecular positive charged types whom tend into offensive molecule wherever EP is robustly negative electrophilic link [25]. Electrostatic potential from free ligands has been calculated and used as a 3D contour to examine the reactive locations of molecules, their stereochemistry, and calculate reaction rates of numerous reactive species, including soft electrophiles and nucleophiles in terms of characteristics from border orbitals (HOMO and LUMO). The interference between HOMO and LUMO values has been plotted in a manner similar to 3D contour to obtain more information on these molecules. The results

TABLE-4
COMPARISON FROM EXPERIMENTAL AND THEORETICAL VIBRATION
FREQUENCIES (cm^{-1}) WITH LIGAND AS WELL METAL COMPLEXES

Compounds	$\nu(\text{OH})$	$\nu(\text{CH})$ aromatic	$\nu(\text{CH})$ aliph.	$\nu(\text{C=N})$	$\nu(\text{N-H})$	$\nu(\text{M-N})$	$\nu(\text{M-O})$
HL	3575* 3434** 0.039***	3021* 3122** -0.033***	2987* 2344** 0.215***	1694* 1756** -0.036***	3243* 3432** -0.058***	—	—
[ReCl ₂ (L) ₂]Cl	—	3026* 3121** -0.031***	2982* 3011** -0.006***	1666* 1755** -0.053***	3240* 3222** 0.005***	534* 555** -0.039***	484*, 423* 400** 0.173***
[PtCl ₂ (L) ₂]	—	3043* 3001** 0.013***	2988* 2900** 0.029***	1635* 1600** 0.021***	3237* 3333** -0.029***	586*, 536* 566** 0.034***	491*, 474* 444** 0.095***
[Pd(L) ₂]	—	3022* 3222** -0.066***	2979* 2900** 0.026***	1676* 1600** 0.045***	3239* 3222** 0.005***	530* 500** 0.056***	480*, 424* 422** 0.120***
K ₂ [CuCl ₂ (L) ₂]	—	3043* 3000** 0.014***	2957* 2900** 0.019***	1634* 1633** 0.0006***	3241* 3222** 0.005***	582*, 536* 555** 0.046***	500*, 474* 444** 0.112***
K ₂ [CoCl ₂ (L) ₂]	—	3023* 3000** 0.007***	2937* 2922** 0.005***	1682* 1650** 0.019***	3240* 3400** -0.049***	534* 500** 0.063***	484*, 423* 488** -0.008***
K ₂ [NiCl ₂ (L) ₂]	—	3021* 3000** 0.006***	2968* 2933** 0.011***	1637* 1600** 0.022***	3236* 3255** -0.005***	580*, 540* 530** 0.086***	490*, 420* 488** 0.004***

*Empirical frequency. **Theoretical frequency. ***Error % because of the main difference in empirical mensuration as well as theoretical treatments from spectrum vibration.

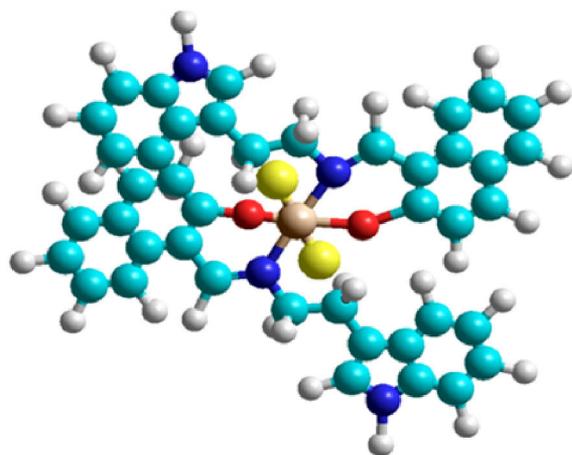
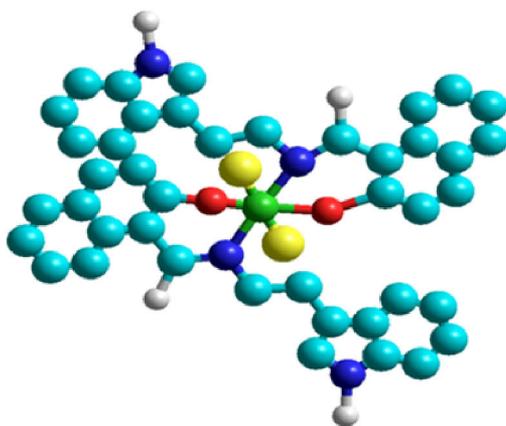
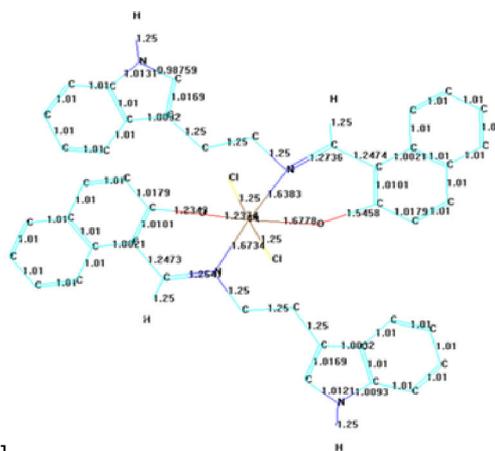
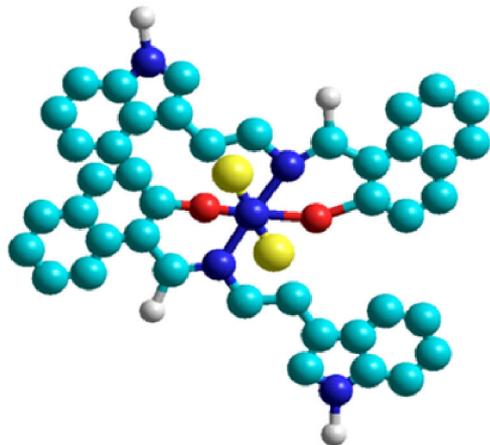
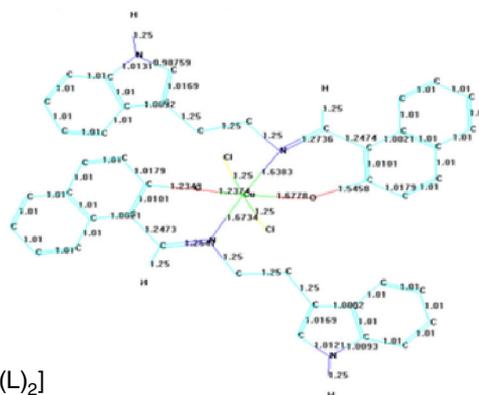
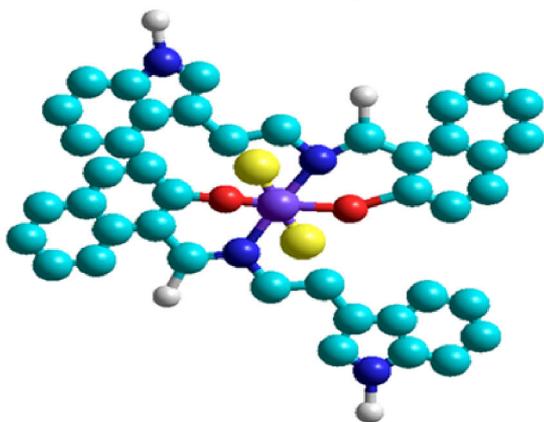
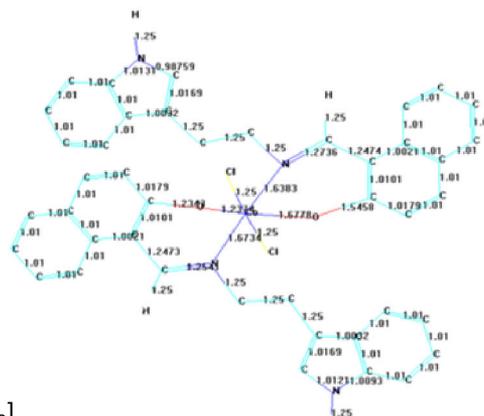
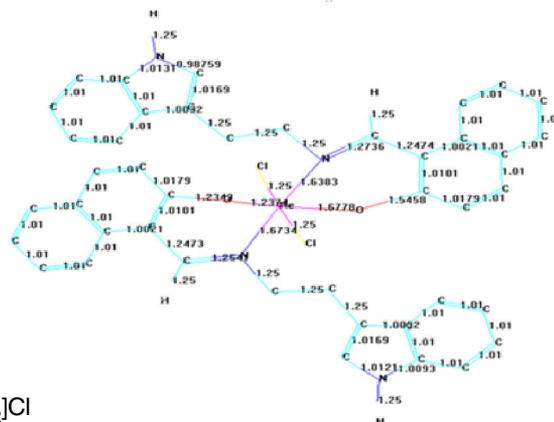
[PtCl₂(L)₂][CuCl₂(L)₂][CoCl₂(L)₂][ReCl₂(L)₂]Cl

Fig. 2. Conformational structures of ligand and its metal complexes

TABLE-5
CONFORMATION ENERGETIC (KJ mol⁻¹) ALSO DIPOLE MOMENT WITH LIGAND ALSO METAL COMPLEXES

Compounds	Binding energy	Heat of fashioning	Electronic energy	Dipole moment (debye)
HL	-3237.3109465	741.1420535	-451373.8437952	3.257
[ReCl ₂ (L) ₂]Cl	-1137.3109465	-1137.3109465	-322137.3109465	1.257
[PtCl ₂ (L) ₂]	-937.3109465	-937.3109465	-113237.3109465	2.570
[Pd(L) ₂]	-837.3109465	-837.3109465	-493237.3109465	2.700
K ₂ [CuCl ₂ (L) ₂]	-37.3109465	-7.3109465	3.2570000	1.200
K ₂ [CoCl ₂ (L) ₂]	-67.3109465	-3.3109465	3.2570000	2.200
K ₂ [NiCl ₂ (L) ₂]	-68.3109465	13.3109465	3.2570000	0.900

TABLE-6
ANTIBACTERIAL EFFICACY DATA OF LIGAND AND ITS METAL COMPLEXES AS INHIBITION ZONE (mm)

Compounds	Bacteria								Fungi							
	<i>Staphyococcus aureus</i>		<i>Bacillus subtilis</i>		<i>Pseudomonas aeruginosa</i>		<i>Escherichia coli</i>		<i>Penicillium expansum</i>		<i>Fusarium graminearum</i>		<i>Macrophomina phaseolina</i>		<i>Candida albicans</i>	
	I	II	I	II	I	II	I	II	I	II	I	II	I	II	I	II
HL	12	–	20	18	12	–	24	12	46	36	–	–	–	–	+++	+++
ReCl ₅	20	10	13	–	15	12	8	–	+++	56	–	–	–	–	+++	+++
H ₂ PtCl ₆ ·6H ₂ O	26	15	–	–	12	–	–	–	38	28	38	33	–	–	–	–
PdCl ₂	12	10	–	–	15	–	–	–	–	–	–	–	–	–	20	10
CuCl ₂ ·2H ₂ O	15	12	23	25	23	18	8	–	–	–	–	–	–	–	–	–
CoCl ₂ ·6H ₂ O	40	25	20	12	16	15	8	12	–	–	–	–	–	–	–	–
NiCl ₂ ·6H ₂ O	30	12	19	24	20	14	24	30	–	–	–	–	–	–	–	–
[ReCl ₂ (L) ₂]Cl	24	–	23	19	24	18	30	12	12	–	12	–	24	20	12	8
[PtCl ₂ (L) ₂]	18	–	23	19	22	15	40	32	23	19	24	14	25	20	23	15
[Pd(L) ₂]	30	25	25	20	28	18	–	28	23	19	25	20	–	–	8	–
K ₂ [CuCl ₂ (L) ₂]	28	22	12	21	12	–	–	–	30	28	30	22	30	20	25	17
K ₂ [CoCl ₂ (L) ₂]	24	20	32	13	22	15	15	22	23	17	19	12	–	–	29	18
K ₂ [NiCl ₂ (L) ₂]	38	30	21	18	28	18	19	8	23	20	–	–	25	14	–	–
Control	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

(I): High concentration; (II): Low concentration; (+++): Strong inhibition

revealed that LUMO from transition metal ion prefers to react for HOMO from nitrogen atoms of azo-Schiff base ligand (Fig. 2).

Microbiological activities: The isolated bacteria were inoculated in tubes for nutrient broth (NB). The classified NB (1 cm³) was homogenized and heated using burners at 45 °C. Homogeneous commentary have been casted to petri plates. Discs of filter paper (dia. 4 mm) were introduced on the discs. After the solidified form of NB cooled and a formed layer of 2 × 10⁻⁵ dm³ of the test compounds was applied. After nursery for 24 h in thermostat at 25-27 °C, inhibition (sterilized) zone diameters (involving disc) have been measured in mm. An inhibition of diameter zone of > 7 mm indicated that the tested compound is effective against bacteria [26]. Antibacterial activity of the synthesized ligand, metal salts and complexes have been screened against Gram-negative bacteria such as *Escherichia coli* and *Pseudomonas aeruginosa* and Gram-positive bacteria such as *Bacillus subtilis* and *Staphylococcus aureus*.

All the metal complexes, metal salts and ligand have been tested for their activity against fungi such as *Penicillium expansum*, *Fusarium graminearum*, *Macrophomina phaseolina* and *Candida albicans*. The results are shown in Table-6.

Conclusion

All compounds were prepared and characterized using spectroscopic techniques such as FT-IR, UV-visible, ¹³C & ¹H NMR, mass and elemental analysis. Theoretical studies of the ligand and its complexes have also been performed using the quantum chemical calculation asymptotic through density func-

tional theory. A good correlation between empirical and experimental results were found. The prepared ligand and its metal complexes have been examined for their anti-bacterial and anti-fungal activities.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

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