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RESEARCH ARTICLE

Synthesis and Biological Study of Schiff–Mannich Base Derived from 2-Mercaptobenzimidazole as Chelated Tridentate Ligand with Some Transition Metal Ions Complexes

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ABSTRACT

To prepare a new ligand, many compounds were used to synthesize Schiff-Mannich base, such as isatin, Para chloro Aniline, 2-mercaptobenzimidazole and indole. The resulting compound 1-((2-((1H-indol-1-ylthio)-1H-benzo[d]imidazol-1-yl)methyl)-3-(4-chlorophenylimino)indolin-2-one (L). (L) was used to create a series of metal ion complexes with Co (II), Ni (II), Cu (II), Pd (II), Pt (IV), and Au (III). C.H.N.S., FTIR, mass spectra UV-ViS, 1H-NMR, 13CNMR, magnetic moment, and molar conductivity were used to characterize all of these compounds. Except for the palladium(II) and gold(III) complexes, all of the produced complexes had an octahedral geometry, according to the data. The antibacterial activity of the produced compounds was tested by using gram-negative and gram-positive bacteria and fungi at a concentration 0.02M. The study showed that cobalt and nickel complexes are the most effective among them. Theoretical study was conducted using the Hyper-chem program to calculate the standard heat of formation and binding energy for all prepared compounds, in addition to calculating the highest occupied molecular orbital by electrons and the lowest unoccupied molecular orbital, in addition to calculating the vibration frequencies for ligand.

Keywords: Antibacterial and antifungal activity, 2-mercaptobenzimidazole, Para-chloroaniline, Schiff-Mannich base, Transition metal complexes

Introduction

The biological activity and pharmacological characteristics of the benzimidazole derivatives have prompted us to look into the coordination actions of benzimidazole derivatives towards transition metal ions. However, bis(benzimidazole) ligands, which indicate a class of aromatic N-donor organic linkers, have a different activity as they can act as bacteriostats or bactericides, fungicides, anticarcinogens, etc.[1]. Mannich base compounds have been utilized as antibacterial[2], antimalarial, antiviral[3], anticonvulsive[4], anti-inflammatories[5], and fungicidal[6] agents.

Schiff base ligands play a role in coordination chemistry because they are capable of creating stable complexes with metal ions[7]. Schiff bases are used in a wide range of fields, including analytical, biological, and inorganic chemistry. They are an essential category of organic substances which are extensively utilized. R-H substrates in Mannich reactions can come from a wide range of structurally diverse compounds.

Depending on whether the active hydrogen atom is on a carbon atom or a heteroatom that may form bonds with sulfur, the amino methylation process may result in the C-, S-, N-, O-, and P-Mannich reactions, nitrogen, oxygen, or phosphorus are all

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examples of elements[8]. The Mannich method is commonly used to generate compounds including nitrogen[9]. The most unexpected parts of chemistry are known as heterocyclic chemistry[10], and heterocyclic compounds are of fundamental relevance in medicinal chemistry[11]. The production of metal complexes with benzimidazole ring with ligands is being studied. As a result of the significance of drugs and their complexes, it was essential to synthesize and characterize certain transition metal substituted benzimidazoles, particularly when it has been reported that the influence of the substitution at 1, 2, and 5-positions is extremely significant to their pharmacologicaleffect[11]. In this research when comparing our study with previous studies, the ligand that was prepared using the drug Sulfabenzamide is a new tri-dentate ligand, in addition to the fact that the complexes prepared from this ligand are new complexes with different geometric shape. The biological activity of all compounds was studied against selected types of bacteria and fungi. The study proved that cobalt and nickel complexes have high biological effectiveness with all types selected (bacteria and fungi) when compared with the same type of bacteria or fungi from previous studies. In addition, our research includes a theoretical study using the Hyper Chem8.0.7 program to calculate a number of factors that show the thermodynamic stability of all prepared complexes when comparing to the ligand. The HOMO, LUMO and vibration frequencies were calculated to compare the accuracy of practical and theoretical results.

Materials and methods

The chemicals utilized in this essay were of the highest quality. The eager 300 elemental analyzer was used to measure the C.H.N.S elemental data. Shimadzu atomic absorption 670 Flam spectrophotometer was used for atomic absorption. Conductivity measurements were collected at concentrations of 10–3 M in complex solution using a PI-700PC GOnDo conduct meter at 25 ˚C in Taiwan. FT-IR spectra of KBr and CsI pellets were obtained using a Shimadzu Fourier-transform 1800 FT-IR spectrophotometer. The absorbance in the UV-Visible region of ethanol solution was measured using a UV-Vis.1800 PC Spectrophotometer Shimadzu. The compounds' ^{1}H- and ^{13}C-NMR spectra were acquired on a nuclear magnetic resonance Varian spectrometer operated by Bruker at 500 MHZ with DMSO solvent and TMS as an internal reference. At 25 ˚C, the magnetic susceptibility of all compounds was measured in a Johnson Mattey balance apparatus. The melting points of the produced compounds were determined using a Gallen Kamp M.F.B-60, and the mass spectra findings were recorded using a network mass selective detector 5973 and measured in the Faculty of Science/University of Tehran laboratory.

Preparation of 2-((1H-indol-1-yl)methylthio)-1H-benzo[d]imidazole (S1)

(0.67 g, 0.004, mol) of 2-mercaptobenzimidazol was dissolved in (5 ml) absolute ethanol, and after completing the dissolution, it was placed in an ice bath in a round flask, and putting excess of formaldehyde, and after 5 minute, (0.585 g, 0.005 mol) of indol and 2 drops of hydrochloric acid were added, then the mixture was placed in a round flask with refluxed stirring for 6 hours. The precipitate was thoroughly washed with distilled water and ethanol[12]. A dry (light orange) precipitate having a melting point of (229–231) ˚C was produced as shown in Fig. 1.

Preparation of 1-((2-(1H-indol-yl)methylthio)-1H-benzo[d] imidazol-1-yl)methyl)indoline-2,3-dione (S2)

In a round bottom flask and using ethanol as a solvent, (1 g,0.003 mol) of **2-((1H-indol-1-yl)methylthio)-1H-benzo [d] imidazole** was dissolved and (0.44 g, 0.003 mol) of istain was also dissolved with excess of formaldehyde in ice bath to it, then two drops of concentrated HCl were added to the mixture, then the mixture was placed on reflux and heated for a period of (6 hours). The ligand of Mannich base is a brown precipitate with a melting point of (201-203) ˚ C and the formula $C_{25}H_{18}N_4O_2S$ that was permitted to dry[12].

Synthesis of 1-((2-((1H-indol-1-ylthio)-1H-benzo[d]imidazol-1-yl)methyl)-3-(4- chloro phenyl imino) indolin-2-one (L)

Using equal mole of 1-((2-(1H-indol-yl)methylthio)-1H-benzo[d]imidazol-1-yl)methyl)indoline-2, 3-dione (Mannich base) (S2) (1g) and parachloro anline (0.25 g) after dissolving them in ethanol. The mixture was added in a round flask. A few drops of glacial acetic acid were added, and the mixture was refluxed for 6 hours until a brownish-black precipitate appeared; the precipitate was rinsed with ethanol, filtered, dried, and its melting point was determined to be 298–300 ˚C, Fig. 1.

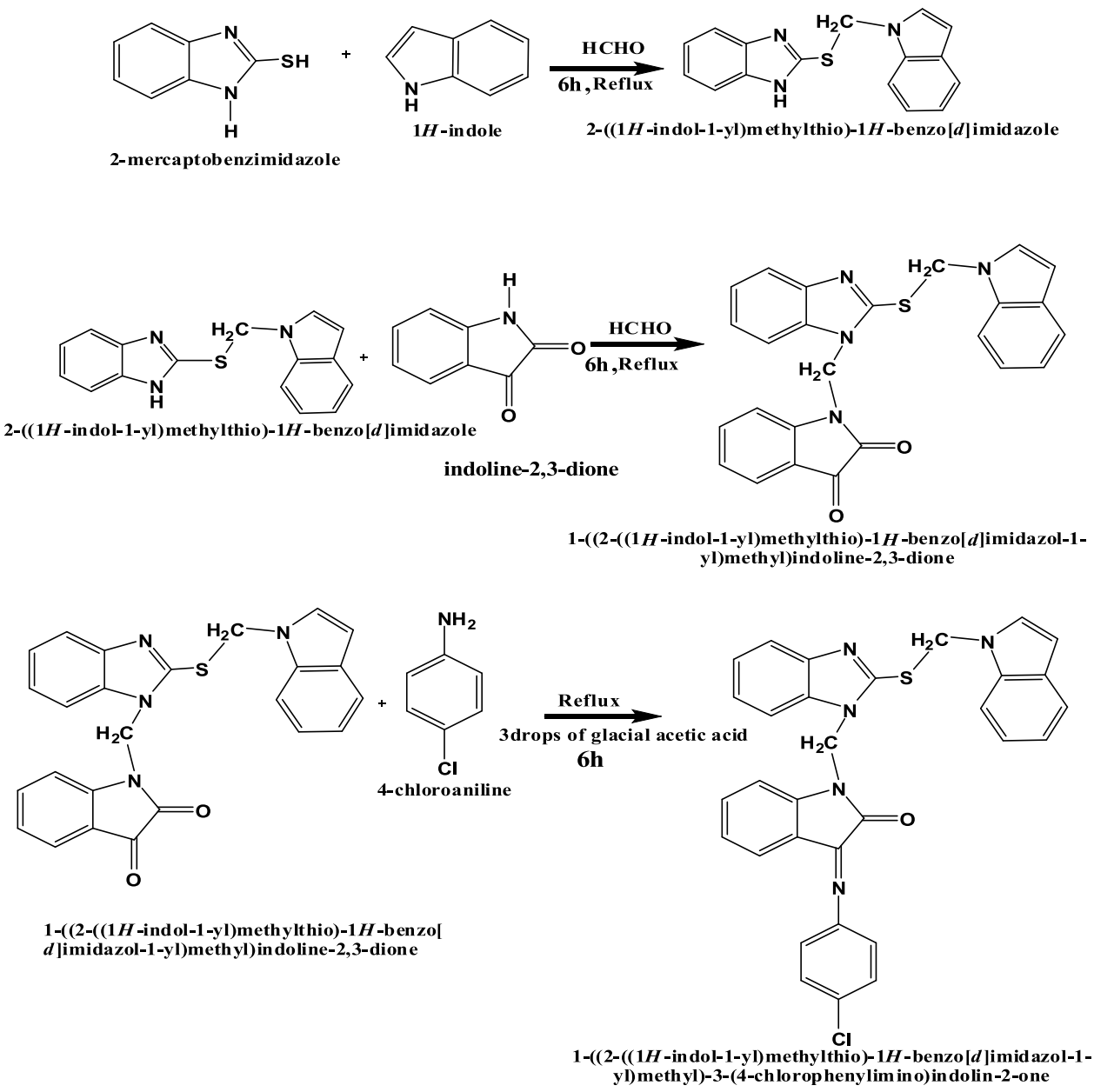

Fig. 1. Synthesis of ligand (L).

Synthesis of ligand complexes

The complexes of the ligand L were prepared in a round flask by dissolving equal mole of ligand (L) and metal salts in ethanol solvent for each of the $CoCl_2.6H_2O$, $NiCl_2.6H_2O$, $CuCl_2.2H_2O$, $PdCl_2$, $H_2PtCl_6.6H_2O$ and $HAuCl_4.H_2O$. Then metal salts were gradually added to the ligands, complexes of different colors were obtained. The mixture was refluxed for 3 hours at a temperature (50) ˚C with continuous stirring, then the precipitate was recrystallized, dried, and diagnostic tests were performed.

Theoretical Treatment: The standard heat of formation and binding energy of the ligand and all produced complexes were determined using the PM3 method for Co(II), Ni(II), and Cu(II) complexes, and the AMBER method for Pd (II), Pt(IV), and Au(III) complexes. The ligands' vibrational frequencies were computed applying the PM3 method, and the findings were compared to the experimental findings.

Antibacterial and antifungal activity

Under aerobic conditions, the well diffusion method was employed to investigate the efficacy

Table 1. The physical properties of color and melting point in addition to the values of C.H.N.S and the percentage of all prepared compounds.

Formula MWt	m.p^{0}C	Color	Yield%	Molar ratio (M:L)	Elemental analysis Calc. (Found) C	H	N	S	Metal% Calc. (Found) M%
$C_{31}H_{22}N_5O_1S_1$(L) 548.06	298-200	brownishblack	68	——	67.93 (68.56)	4.01 (4.89)	12.77 (11.89)	5.84 (6.04)	——
$C_{31}H_{26}N_5O_3S_1Co$ 712.8	276-278	Pale grey	73	(1:1)	52.17 (53.11)	3.64 (3.69)	9.81 (10.12)	4.49 (5.19)	8.26 8.89
$C_{31}H_{26}N_5O_3S_1Ni$ 747.67	255-257	Light green	80	(1:1)	49.75 (50.67)	3.47 (3.53)	9.36 (9.69)	4.28 8.22	7.84
$C_{31}H_{28}N_5O_4S_1$ Cu 735.51	Over300	Green	75	(1:1)	50.61 (49.33)	3.8 (4.71)	9.52 (10.12)	4.36 (5.3)	8.63 9.06
$C_{31}H_{24}N_5O_2S_1Pd$	Over300	Black	70	(1:1)	47.87 (48.47)	3.08 (3.79)	9.01 (9.79)	4.12 (4.87)	13.68 14.09
$C_{31}H_{24}N_5O_2S_1$ Pt 935.99	233-235	Brownish	66	(1:1)	39.78 (40.34)	2.51 (2.67)	7.48 (7.69)	3.42 (4.18)	20.84 —-
$C_{31}H_{26}N_5O_3S_1$ Au 920.9	120-122	Brown	76	(1:1)	40.39 (41.22)	2.82 (3.00)	7.6 (8.45)	3.48 (4.14)	21.38 22.14

of ligand (L) and their metal complexes against pathogenic bacteria. Mueller-Hinton agar was used to test the inhibitory activity against all pathogenic bacteria. After cultivating each indicator microbe (*Escherichia coli, Pseudomonas aueruginosa, Staphylococcus aureus, Streptococcus, and Candida albicans*) in a nutrient broth, agar plates were injected with (1.5 * 108 (CFU)/ ml for bacteria and 1.5 * 106 (CFU)/ ml for mold and yeast, in compared to 0.5 McFarland tube. Wells (6 mm) were cut in Mueller-Hinton agar and 100 microliter of ligand and their metal complexes have been added to each well. Plates containing bacteria were cultured at 37°C for 24 hours. For the fungus species, however, the plates were incubated at 28°C for 72 hours. To measure activity, the diameter of inhibitory zones (mm) was used[13].

Results and discussion

In this research, many complexes of different colors were prepared and studied by some spectroscopic methods in addition to physical methods to determine their geometric shapes and type of atoms coordination with the central metal ion. In Table 1, many properties related to the ligand and its complexes have been determined, including color, molecular weight, and the calculation of the proportion of elements C.H.N.S, in addition to calculating the proportion of metals using the atomic spectrum method.

Transforms spectroscopy (FT-IR) of ligand (L) and its metal complexes

The FT-IR spectrum for free ligand revealed seven main bands: 1732, 1599, 1612, 1176, 760 cm^{-1}, and 2854, 2966 cm^{-1}, which corresponded to vC=O[12], C=N$_{ring}$, C=N$_{schiff}$[13], CSC, CS, and CH$_2$-N[14], Fig. 2. When coordinated with metal ions, some of these peaks shifted to higher or lower frequencies, while others did not change because there was no displacement in them, indicating that bonding did not occur through them, including the azomethin group. The frequency changed at the range 2894 to 2981cm^{-1} of cobalt, Fig. 3, nickel, copper, palladium, platin, and gold complexes were reported when attaching to the nitrogen atom of Mannich base. In all produced complexes, the bands of vCSC and vCS group moved according to the frequencies (1176, 1186, 1192, 1219, 1196, 1180, 1189) cm^{-1} and (744, 739) cm^{-1} of CSC, respectively. In addition, there was a distinct shift in the carbonyl band for all compounds (57, 19, 11, 10, 16, and 31) cm^{-1}. These band shifts show the presence of ligand coordination via the Mannich group's nitrogen, the CS group's sulfur, and the carbonyl group as tridentate ligand. Medium bands appeared at (597–540) and (470–416) cm^{-1}, which might be attributed to vM-N and M-S for complexes[13,14]. Table 2. shows additional bands.

Uv-vis spectra, magnetic susceptibility and molar conductivity

In ethanol solvent, the electronic spectra of all prepared compounds were recorded. In Schiff-Mannich ligand (L) the bands at 29850, 37313 cm^{-1} are attributed to n $\rightarrow \pi^*$ and $\pi \rightarrow \pi^*$ transition respectively, Fig. 4. All electronic transitions can be observed in Table 3.

In the **cobalt complex**, bands appeared at absorbers (10471, 18115 and 23640) cm^{-1}, which

Table 2. Infrared spectrum data of the ligand and its metal complexes (cm^{-1}).

Comp.	νC=O	νC=N ring	νC=N	νCSC	νCS	νCH_2-N	νM-N	νM-S	νM-Cl
L	1732	1599	1612	1176	760	2854 2966	——	——	——
CoL	1789	broad	1608	1186	744	2894 2906	551	416	343 369
NiL	1751	1594	1609	1192	739	Broad 2943	563	470	
CuL	1721	1599	1610	1219	744	2868 2943	543	420	347
PdL	1720	1591	1615	1196	744	2840 2920	540	432	345
PtL	1716	broad	1616	1180	744	2835 2958 2924	597	428	331
AuL	1701	broad	1608	1189	744	2823 2981	559	447	322

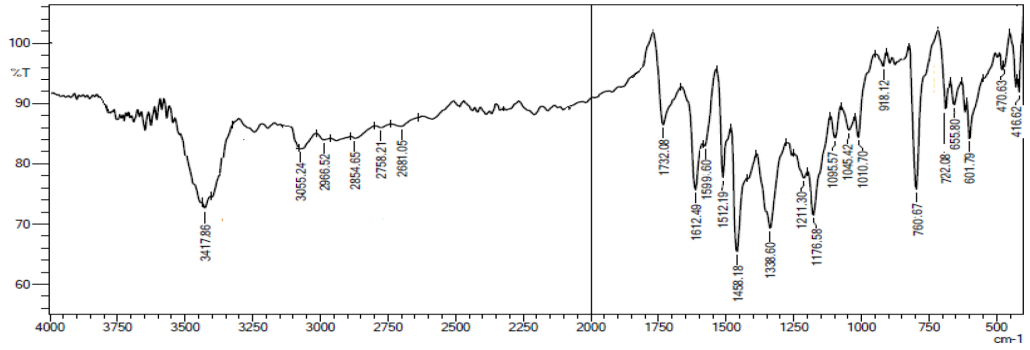

Fig. 2. FT-IR spectrum of L.

Table 3. UV-vis spectrum, conductivity and magnetic sensitivity of organic ligand (L) and their complexes.

Comp.	Absorption n.m	Absorption Cm^{-1}	Assignments	μe_{eff} B.M.	Conductivity $\mu S.cm^{-1}$	Suggested geometry
L	335	29850	n→ π^*	…..	….	——
	268	37313	$\pi \rightarrow \pi^*$			
CoL	955	10471	$^4T1g \rightarrow {}^4T_2g$	3.97 (3.87)	19	Octahedral
	552	18115	$^4T_1g \rightarrow {}^4A_2g_{(f)}$			
	423	23640	$^4T_1g \rightarrow {}^4T_1g$ (p)			
	318	31446	IL → CoCT			
	305	32786	IL → CoCT			
NiL	982	10183	$^3A_2g \rightarrow {}^3T_2g$	2.95 (2.82)	20	Octahedral
	644	15527	$^3A_2g \rightarrow {}^3T_1g$ (f)			
	376	26595	IL → NiCT			
CuL	875	11428	$^2Eg \rightarrow {}^2T_2g$	1.78 (1.73)	17	Octahedral
	373	26809	IL → CuCT			
	353	28328	IL → CuCT			
	251	39840	IL → CuCT			
PdL	421	23759	$^1A_1g \rightarrow {}^1B_1g$	0	72	Square planar
	358	27932	$^1A_1g \rightarrow {}^1Eg$			
	242	41322	IL → PdCT			
PtL	898	11135	$^1A_1g \rightarrow {}^3T_2g, {}^3T_1g$	0	78	Octahedral
	430	23255	$^1A_1g \rightarrow {}^1T_1g$			
	386	33557	$^1A_1g \rightarrow {}^1T_2g$			
	246	40650	IL → PtCT			
AuL	448	22321	$^1A_1g \rightarrow {}^1B_1g$	0	166	Square planar
	362	27624	$^1A_1g \rightarrow {}^1Eg$			
	239	41841	IL → AuCT			

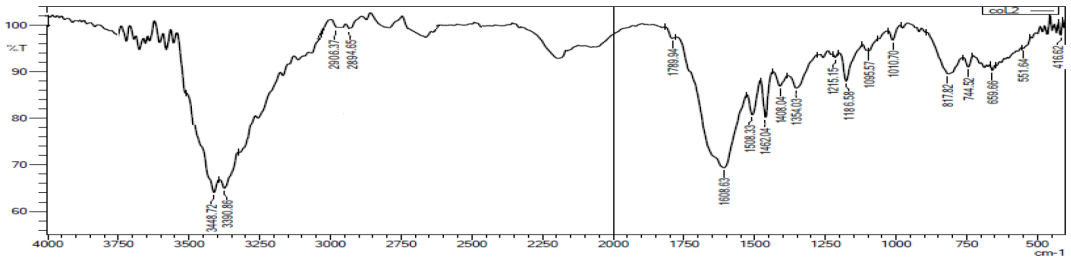

Fig. 3. FT-IR spectrum of CoL.

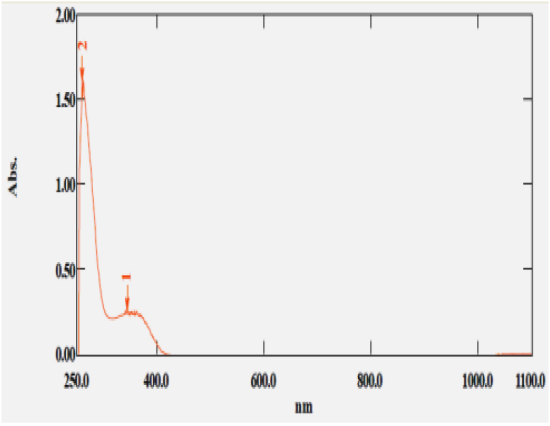

Fig. 4. UV-Vis spectrum of L.

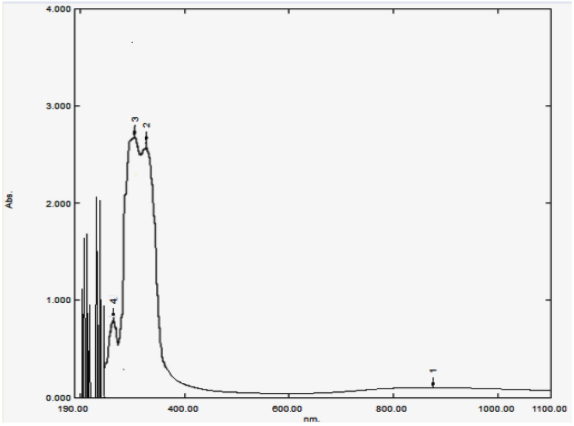

Fig. 5. UV-Vis spectrum of CuL.

are due to electronic transitions $^4T_1g \rightarrow {}^4T_2g$, $^4T_1g \rightarrow {}^4A_2g$ (F) and $^4T_1g \rightarrow {}^4T_1g$ (p) transitions .The appearance of these peaks in the above locations indicates that the complex is octahedral[15]. The presences of other bands are due to the charge transfer from the ligand to the metal at 31446 and 32786 cm^{-1}. Magnetic moment, 3.97 B.M. The conductivity value (19 $\mu S.cm^{-1}$) shows that the complex is not conductive[16]. Transitions and suggested geometry can be seen in Table 3.

The light green **nickel complex** spectrum shows absorption bands at 10183, and 15527 cm^{-1} is due to $^3A_2g \rightarrow {}^3T_2g$, and $^3A_2g \rightarrow {}^3T_1g_{(f)}$ in addition to the appearance of the charge transition band at 26595 cm^{-1}, which indicates the occurrence of the transition from intra ligand to Ni. These electronic transitions indicate that the complex has an octahedral geometry[15]. The value of magnetic moment indicates that the complex is high -spin, while the value of conductivity indicates that the complex is non-ionic[16], Table 3.

In the spectrum of the **copper complex**, which is green in color, a broadband electron transition at 11428 cm^{-1} is attributed to the transition $^2Eg \rightarrow {}^2T_2g$, Fig. 5. Other bands at 26809, 28328 and 39840 cm^{-1} are due to intra ligand charge transfer from ligand to metal which gives an octahedral geometry of Cu (II) complex[17]. The value of the magnetic sensitivity was recorded as (1.78) BM, which indicates the presence of one electron, in addition to the fact that the practical value is higher than the theoretical one, which indicates the occurrence of spin orbital coupling. In addition, the conductivity value at 17 $\mu S.cm^{-1}$ indicates that the complex is non-ionic[18], Table 3.

In the **palladium complex**, the following two bands appeared at 23759 and 27932 cm^{-1}, which belong to transitions $^1A_1g \rightarrow {}^1B_1g$ and $^1A_1g \rightarrow {}^1Eg$, respectively. These transitions confirm that the complex has a square planar geometry[19]. The value of the magnetic sensitivity is recorded as zero, and this value indicates that the complex is low spin. The value of conductivity, it indicates that the complex is conductive in a ratio of (1:1)[20].

In the **complex spectrum of platinum (IV)** two bands appeared at 23255 and 27624 cm^{-1} are assigned to $^1A_1g \rightarrow {}^1T_1g$ and $^1A_1g \rightarrow {}^1T_2g$, transitions. These bands confirm that this complex is octahedral[20]. Forbidden band at (12091) cm^{-1} is assigned to $^1A_1g \rightarrow {}^3T_2g$, ^3T_1g. Magnetic moment, (0) B.M this value detects that the complex is low spin. The value of conductivity is (78$\mu S.cm^{-1}$), it indicates that the complex is conductive in a ratio of (1:1)[21].

The **gold complex** shows two bands at 22321 and 27624 cm^{-1} assigned to $^1A_1g \rightarrow {}^1B_1g$, and

Table 4. ^{1}H- and ^{13}C-NMR of new ligand (L).

	^{1}HNMR		^{13}CNMR
Founctional groups	δ ppm	Founctional groups	δ ppm
DMSO (solvent)	2.51	DMSO (solvent)	39.13-40.79
L			
H_2O	3.62	C = N of benzamidazole ring	141.02
Ar-H	7.22-7.91, 16H, Multiplet	C=N of imine ring	165.71
CH_2-N (Mannich) 2 groups	5.11,5.64,2H Douplet	CH_2-N (Mannich) 2 groups	61.87
	5.70,5.87, 2H Douplet		65.71
C-H of benzamidazole ring	6.22,7.13, 1H, Duplet	C = O group	169.64
		C-Ar	111.38–132.55
		C-Cl	133.44

$^{1}A_1g \rightarrow {}^{1}Eg$ transitions, which indicate this complex has a square planar geometry[22]. Magnetic moment (0) B.M. Conductivity measurement (166) μS.cm^{-1} shows that the complex is ionic in a ratio of (1:2)[23]. Transitions and suggested geometry can be seen in Table 3.

All forms of the proposed complexes are shown in Fig. 6.

^{1}H-NMR and ^{13}C-NMR Spectra of Ligand (L)

Another way to identify ligand is proton nuclear resonance spectroscopy. All chemical shifts of the ligand are shown in Table 4. The ^{1}H-NMR was made at 500 MHz and using DMSO-d_6 solvent .The spectrum of Schiff- Mannich-base (L) shows singlet absorption peaks at 2.51 and 3.62 ppm which belong to the solvent and water respectively[24]. The appearance of multiple other peaks in the range 7.22–7.91 ppm, which are related to the protons of the aromatic ring in the ligand. δ511,5.64 and δ5.70,5.87 ppm this bands due to methylene groups of Mannich base[25]. In addition, there are other peaks that can be noted in Table 4. As for the ^{13}C-NMR spectrum, the important signals appeared at 141.02, 165.71, and 169.64 ppm, which belong to the carbons of C = N of benzimidazole ring, C = N of imine group and carbonyl group respectively. The signals observed between 111.38–132.55 ppm are due to carbon aromatic phenyl ring. There are other peaks that can be seen in Table 4.

Mass spectra

The mass spectrum **of 1-((2-((1H-indol-1-ylthio)-1H-benzo [d] imidazol-1-yl)methyl)-3-(4-chloro phenyl imino) indolin-2-one (L)** shows an insignificant intensity peak at 547.1 m\z, which occurs by the molecular ion of the empirical formula. ($C_{31}H_{22}N_5OSCl$).The fragment peak at 144 m\z [$(C_8H_4N_2O)^+$,100)] it represented the base peak. Other fragments peaks at 417 m\z [$(C_{22}H_{14}N_4OSCl)^+$,30)],255 m\z [$(C_{14}H_8N_2OCl)^+$,8)], 131 m\z [$(C_9H_9N)^+$,23], 114 m\z [$(C_7H_6NS)^+$,26], 112 m\z [$(C_6H_6Cl)^+$,18], 96 m\z [$(C_4H_4N_2O)^+$,20], 78 m\z [$(C_6H_6)^+$,21], and 73.9 m\z [$(CH_2N_2S)^+$,52].

The molar ratio method

At the maximum wavelength, the ratio of M to L in solution state has been found using molar ratios method at concentration 1 $\times$ 10^{-3} M of all the prepared complexes. The volume of the metal was fixed and the volume of the ligand was changed from 0.25–3 ml by increasing 0.25 ml. The absorbance was fixed at 0.63 for cobalt, 0.43 for nickel, 0.58 for copper, 0.69 for palladium, 0.412 for platinum, and 0.625 for gold. The results proved, through drawing plots shown in Fig. 7 below, that the ratio of the metal to the ligand is (1:1).

Antibacterial and antifungal activity

The biological activity was studied, which includes selected types of bacteria and fungi on all the prepared compounds (ligand and its complexes) with the following types of positive and negative bacteria and fungi *(Staph, streptococcus E-coli, pseudomonas aueruginosa*) and fungi (*candida*) at a concentration of 0.02 M, Table 5. For each treatment, the diameter of the zone of inhibition (mm) including the diameter of the disc was measured. The drug was used as a standard reference (amoxicillin and fucanazole) in comparing the results with for bacteria and fungi, of all prepared compounds. The Co(II) and Ni(II) complexes outperformed the ligand,other complexes and drugs in terms of activity against all species of bacteria and fungi[13]. The chelating mechanism is responsible for these increases in complex activity[26].

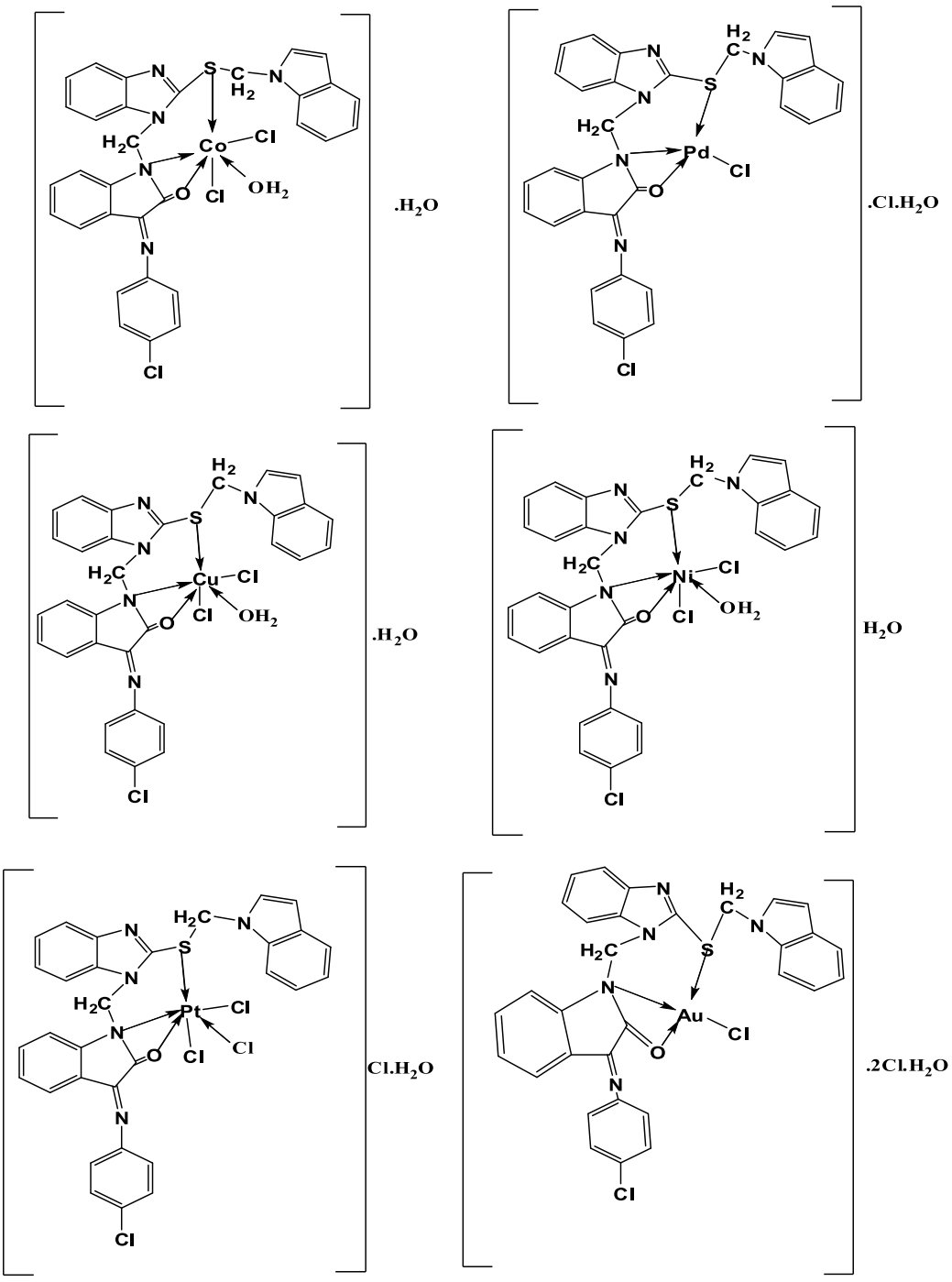

Fig. 6. The proposed geometry of the prepared complexes.

Theoretical study

The vibration spectrum of the L was theoretically calculated using the Hyperchem program, and when comparing the results of the theoretical and practical bands, we found that they were close to each other, Fig. 8. The standard heat of formation and binding energy of complexes as well as the ligand(L), were determined using the HyperChem-8.0.7 program. Because of the presence of coordination from multiple sides, the complexes were shown to be more stable than the Schiff-Mannich base ligand as shown in Table 6.

The electrostatic potential, highest occupied molecular orbital & least unoccupied molecular orbital were calculated to find out the compatible sites in

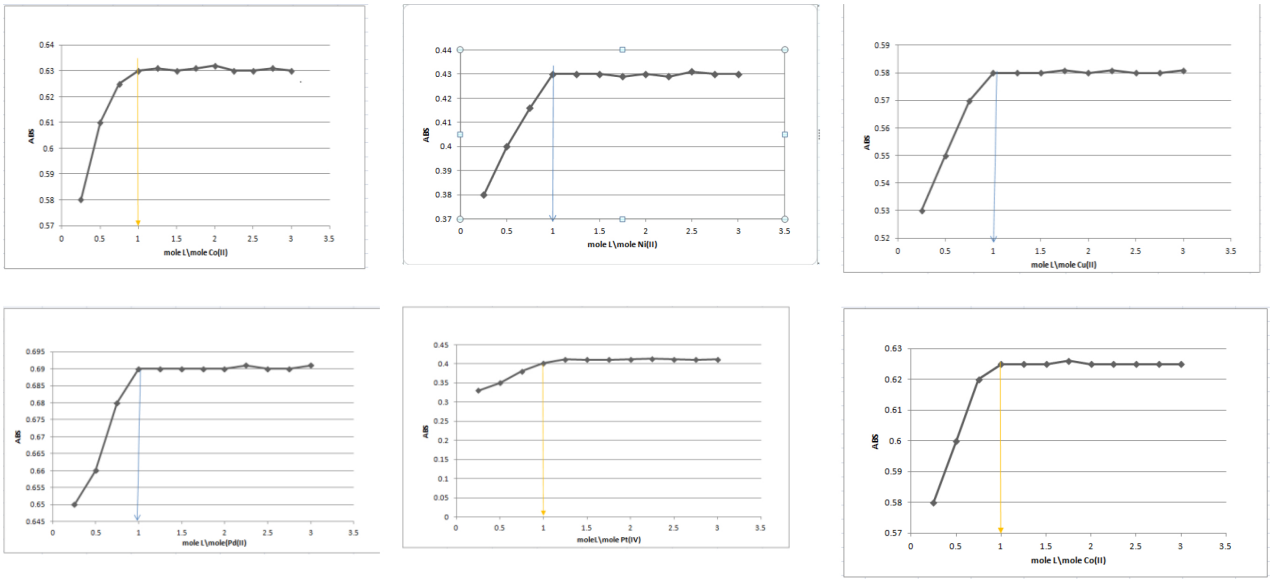

Fig. 7. A curve between absorbance and Ratio mole L\mole M.

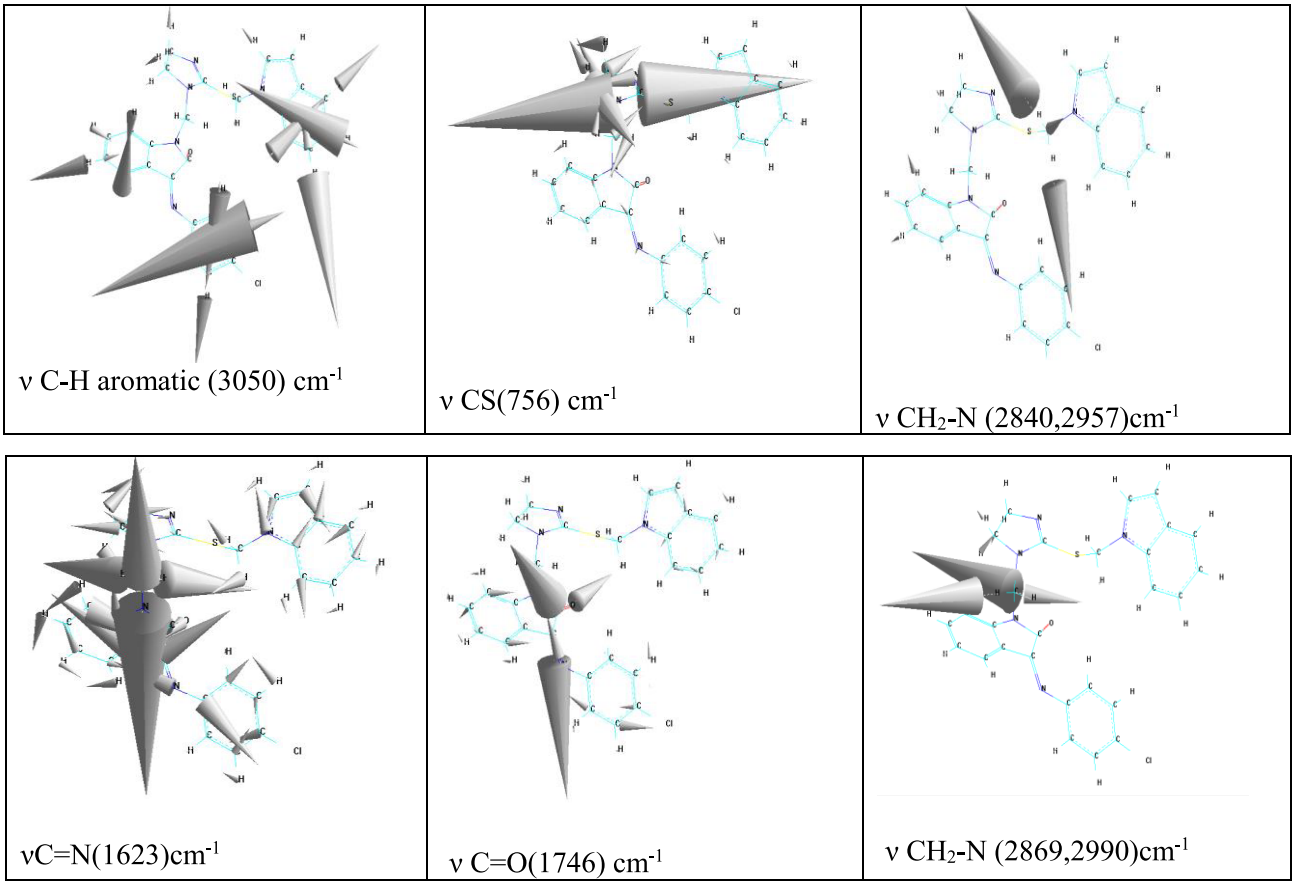

Fig. 8. The vibrational frequencies of L using Hyper Chem-8.0.7 program.

Table 5. The biological activity of all prepared compounds at a concentration of 0.02 M in DMSO.

		Types of bacteria and fungi				
		Gram negative		Gram positive		fungi
	Compounds	*Staph*	*Streptococcus*	*E.coli*	*Pseudomonas aueruginosa*	*Candida*
1	CoL	26	25	28	26	33
2	NiL	24	28	21	24	30
3	CuL	11	10	11	11	19
4	PdL	9	9	9	10	13
5	PtL	9	10	11	10	12
6	AuL	23	19	20	18	17
7	DMSO	-	-	-	-	-
8	Schiff-Mannich (L)	9	10	10	13	10
9	Amoxicillin	10	9	10	9	—
10	Fucanazole					12

(-): Which mean negative.

Table 6. The table shows the standard heat of formation and binding energy for all the prepared compounds, along with calculating the magnetic moment for them by using PM3 and AMBER methods.

	PM3			AMBER	
Comp.	ΔH°_{f}	ΔE_b	μ	$\Delta E_b = \Delta H^{\circ}_{f}$	μ
L	24.3498701	-89.3487901	1.43	——	—-
CuL	-390.4560982	-9800.657809	2.89	—-	—-
CoL	-858.6667773	-7983.879032	5.11	——	—
PdL	——	——-	——	172.435	—-
PtL	——	——-	——	329.1897	—
AuL	——	——	——	86.5567	—-

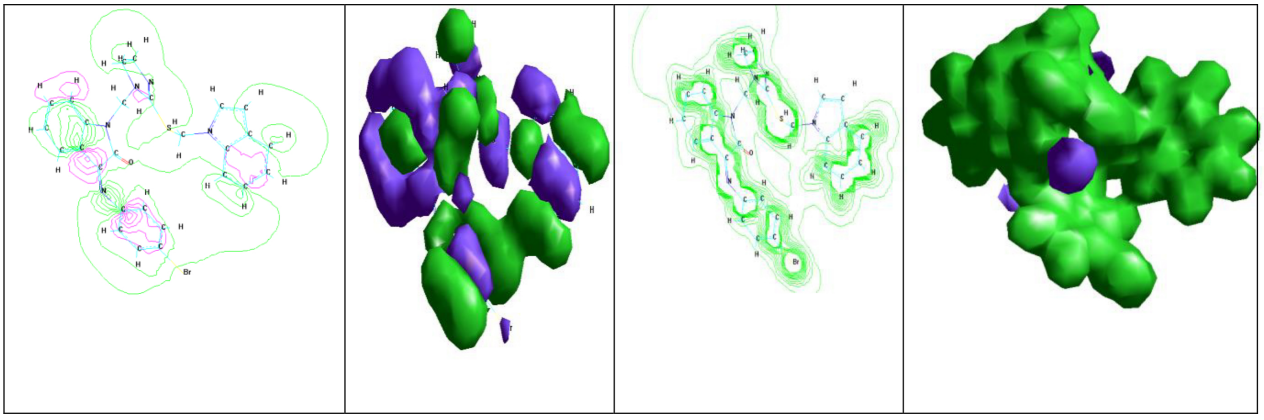

Fig. 9. Areas of HOMO, LUMO, and electrostatic potential in different dimensions.

the ligand that carry high electron density to form the coordination complex, Fig. 9.

Conclusion

The conventional method was utilized successfully to synthesize a new ligand Schiff-Mannich base (L) derived from 2-Mercaptobenzimidazole. A series of multivalence complexes (II, III, and IV) were synthesized and characterized utilizing a variety of physical and spectroscopic techniques. The results showed that cobalt, nickel, copper and platinum complexes have octahedral geometry, but palladium and gold complexes have square planar geometry. The biological activity of two types of positive bacteria, two types of negative bacteria, and one type of fungus were studied. The results showed that cobalt and nickel complexes have an effectiveness superior to that ligand, other complexes, and controls. The theoretical treatment, which estimated the (ΔHf ^{0}) and (ΔE^{0}) using program hyperchem 8.0.7, revealed that the complexes are more stable than organic free ligand. The HOMO and LUMO sites showed the important

sites in ligand molecule on which the electronic density is concentrated, thus the identifying the possible atoms the atoms through which coordination with metal ion is likely to occur.

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Author's declaration

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Furthermore, any Figures and images, that are not ours, have been included with the necessary permission for republication, which is attached to the manuscript.
- No animal studies are present in the manuscript.
- No human studies are present in the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at University of Baghdad.

Authors' contribution

Sh. R.B. suggested and planned the research idea, revision and proofreading. Th Q.S designed, carried out the experiments and acquisition of data, both authors contributed in the analysis and discussing of the results and writing the manuscript.

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تحضير ودراسة بايولوجية لقاعدة شف-مانخ المشتقة من ٢-مركبتوبنزميدازول كليكاند مخلبي ثلاثي السن مع معقدات بعض الايونات الفلزية الانتقالية

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الخلاصة

لتحضير الليكاند الجديد هناك العديد من المركبات التي استخدمت لتحضير قاعدة شف-مانخ منها (ازتين,بارا-كلورو اثيلين,2-مركبتوبينزامايدازول والانيدول) والمركب الناتج هو:

(L1-((2-((1H-indol-1-ylthio)-1H-benzo[d]imidazol-1-yl)methyl)-3-(4-chlorophenylimino)indolin-2-one (L). تم استخدامة لتحضير سلسلة من معقدات الايونات المعدنية مع الكوبلت ثنائي التكافؤ , النيكل ثنائي التكافؤ, النحاس ثنائي التكافؤ ,البلاديوم ثنائي التكافؤ, البلاتين رباعي التكافؤ والذهب ثلاثي التكافؤ. تم تشخيص المعقدات الناتجة بعدة فحوصات وهي التحليل الدقيق للعناصر،طيف الاشعة تحت الحمراء، طيف الاشعة فوق البنفسجية- المرئية , طيف الكتلة،طيف الرنين النووي المغناطيسي للبروتون1والكاربون13، العزم المغناطيسي, والتوصيلية المولارية.

و قد أظهرت الفحوصات ان جميع المعقدات بأستثناء معقدات ايون البلاديوم الثنائي والذهب الثلاثي انها ذات تركيب ثماني السطوح. وبالاعتماد على البيانات المستخلصة من التجارب عندما تم فحص المعقدات مع بكتريا غرام الموجبة وبكتريا غرام السالبة والفطريات بتركيز 0.02 مولاري فقد أظهرت الدراسة ان معقدات الكوبلت و النيكل هي اكثر المعقدات فعالية بين باقي المعقدات المحضرة.

اما الدراسة النظرية فقد تمت باستخدام برنامج Hyperchem 8.0.7 و قد تم حساب كل من حرارة التكوين و طاقة التأصر لكل المركبات المحضرة بالإضافة الى حساب طاقة HOMO و طاقة LUMO و ترددات الاهتزاز لليكاند.

الكلمات المفتاحية: فعالية المضادات البكتيرية والمضادات الفطرية، 2-مركبتوبينزامايدازول، بارا-كلوروانيلين، قاعدة شف-مانخ، معقدات المعادن الانتقالية.