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Original Article

Synthesis and Biological Study of Some Transition Metal Ions Complexes of Schiff-Mannich Base Derived from 2-Amino-5-Mercpto-1,3,4 Thiadiazole

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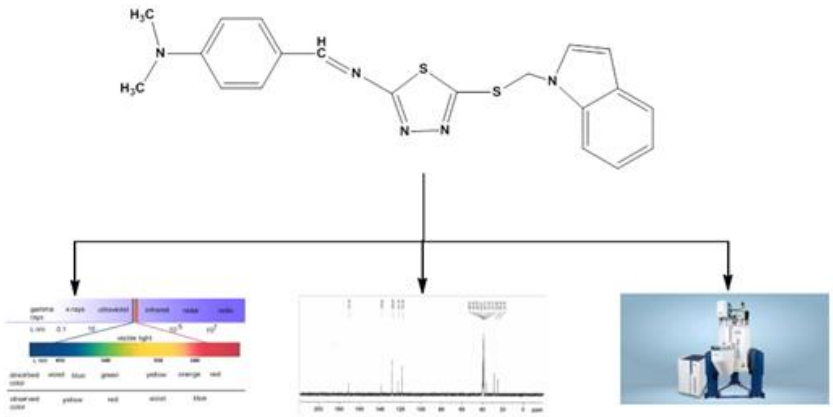
ABSTRACT

The Schiff-Mannich base was derived from 1,3,4 thiadazole prepared by combining of 2-amino-5-mercapto-1,3,4 thiadazole and 4-N,N-dimethyl benzaldehyde with indol. The result compound was 5-((1 H-ind ol -1-yl) methylthio)-N-(4-(dimethylamino)benzylidene)-,1,3,4-thiadiazol-2-amine(L), coordinated with six metal ion Co(II), Ni(II), Cu(II), Pd(II), Pt(IV), and Au(III). The ligand (L) has been characterized by using the following techniques, C.H.N.S, FT-IR, UV-ViS, ^{1}H-NMR, and ^{13}C-NMR. In addition, the measurement of (atomic absorption spectra, magentic susceptibility, and molar conductivity) was used when diagnosing the complexes. The experimental results showed that the ligands coordinated as tri-dentate with metal ions. The antibacterial and antifungal activity of all complexes were studied against *Staphylococcus aureus* and *Bacillus subtilis* as a model of gram-positive, as well as *E-coli* and *Klebsiella pneumoniae* as a gram-negative at a concentration of 0.02 M. Likewise, the effectiveness of the prepared compounds was determined in inhibiting selected types of bacteria and fungi. The results showed that the prepared metal complexes and ligand are more effective than the standard drug in bacteria and fungi. The metal to ligands ratio was determined by the molar ratio method and showed the metal interaction with the ligand proportion (1:1). Also, the compounds prepared were studied in gas phase by using the hyper-chem8.0.7 program. Through this program, the heat of formation, binding energy, HOMO and LUMO, and the electrostatic potential in addition to the infrared vibration of the ligand were calculated.

GRAPHICAL ABSTRACT



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Introduction

Thiadiazole is a five-membered heterocyclic ring that is found naturally in plants and animals, consisting of sulfur, two nitrogen atoms, two carbon atoms, and two double bonds represented by the N=C=S bond responsible for its pharmacological activity [1]. 1, 3, 4-thiadiazole has different applications used as anti-tumor drugs and some of their derivatives were used as carbonic anhydrase inhibitors and antiparkinsonian agents [1], anti-tubercular [2], anticonvulsant [3], hypoglycaemic, CNS depressant [4], etc. Greater *in vivo* stability and non-toxicity for the higher vertebrates, such as humans, are results of this ring system. Due to their numerous uses as antioxidant, catalysts, medicines, crystal engineering, and anticorrosion agents, Schiff base ligands and their transition metal complexes have been well studied [5, 6] for their synthetic adaptability, selectivity, and sensitivity to the central metal atom structural resemblances to naturally occurring biological compounds and the presence of the azomethine group (-N=CH) [7]. Schiff bases are extensively studied due to their ease in the formation of the stable complexes with the majority of transition metal ions, complexes produced from 1,3,4-thiodaizole play a significant role in coordination chemistry [8]. Many biologically important Schiff bases and their metal complexes have been reported in literature possessing, analytical, industrial [9], biological [10] clinical, biochemical, antimicrobial, anticancer, antibacterial, antifungal, and antitumor activity [11, 12] in addition to their important roles in ranging from anticorrosion [13], soil treatment agents, and medicinal agents. The effective catalysts are Schiff base complexes with two or more metal centers [14]. It is also well-known that the biological activity of a ligand is increased and the cytotoxic effects of the metal ion and ligand are reduced when a ligand is coordinated to a metal ion [15]. This investigation focuses on the biological action of Schiff base, its metal complexes, and their production.

Materials and Methods

In this article, the chemicals were used of the highest purity. The C.H.N.S elemental data were measured by eager 300 elemental analyzer. The metal contents were carried out by using Shimadzu atomic absorption 670 Flam spectrophotometer. Conductance data were obtained in 10^{-3} M in DMF solution of the complexes by using WTW conduct meter at 25 °C. Infrared spectra were measured by using Shimadzu and Perkin Elmer FT-IR spectrophotometer by using KBr and CsI pellets. The absorbance in the UV-Visible region was recorded in ethanol solution by using UV-Vis.1800 PC Shimadzu Spectrophotometer. The ^{1}H, ^{13}C-NMR of the compounds were recorded on a Fourier transform Varian spectrometer operating Bruker at 500 MHZ employing DMSO-d_6 solvent and TMS as an internal reference. In a device, Balance of Johnson Mattey, the magnetic susceptibility of all complexes was measured at 25 °C. The melting points of all prepared compounds were measured by Gallen kamp M.F.B-60.

Ligand preparation steps

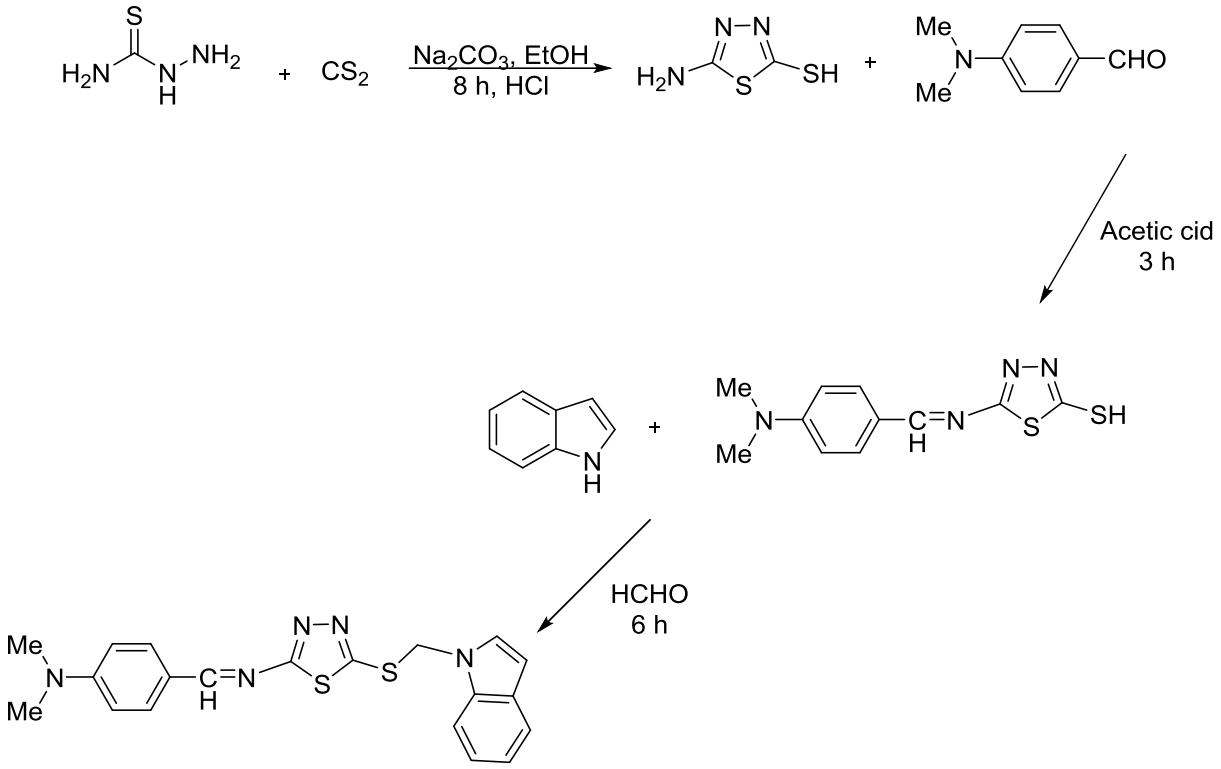
Preparation of 5-((1 H-indol-1-yl)methylthio)-N-(4-(dimethylamino)benzylidene)-,1,3,4-thiadiazol-2-amine(L)

Steps to prepare the new ligand are displayed in (Scheme 1). In 50 mL of absolute ethyl alcohol, 0.02 mol of thiosemicarbizide and 0.02 mol of sodium hydroxide were dissolved. Next, 0.062 mol of carbon disulfide was gradually added to this solution. The mixture was reflux with heating for 8 hours. A greenish-yellow precipitate was produced after carefully concentrating the mixture and acidifying it with hydrochloric acid 10% (HCl). After filtering and washing with cold water, the precipitate was recrystallized with ethanol to produce 2-amino-5-mercapto 1,3,4 thiadazole ($C_2H_3N_3S_2$) (S_1) the precipitate's color was yellowish-white crystals, m. p. 229–231 °C, yield 76%.

Then, in round flask, 0.1 mol of (S_1) and 0.1 mol of (p-(dimethyl amino benzaldehyed) were added after dissolving in ethanol, and then 3-4 drops of

glacial acetic acid was added and the mixture was heated under reflux for 3 hours. The result (S_2) was concentrated and the orange crystals separated was filtered and recrystallized from ethanol. Yield 66 %, m p 173-175 °C.

After preparing (S_2) and using ethanol, 0.1 mol of it was dissolved with 0.003 mol indol. The mixture was heated with the addition of drops of formaldehyde. Under reflux and heating for 6 hours, the dark orange ligand precipitated which separated directly and recrystallized by using ethanol (Scheme 1).



Scheme 1: Steps to prepare Schiff-Mannich ligand (L)

Preparation of complexes

In absolute ethanol, the complexes were prepared by the reaction 1 mmol of the following metal ions with valences II, III, and (IV), ($CoCl_2.6H_2O$), ($NiCl_2.6H_2O$), ($CuCl_2.6H_2O$), ($PdCl_2$) ($H_2PtCl_6.6H_2O$), and ($H_2AuCl_4.H_2O$) with the ligand (1 mmol) in 1:1 ratio and refluxed for 3 hours, and then the precipitate has been filtered and rinsed many times with ethanol. The color solid complexes were formed after evaporation the solvent. Table 1 presents some physical properties of ligand and its complexes.

Computational chemistry

Computational chemistry is one of the chemical applications to solve chemical problems by using mathematical applications based on molecular shape (sample molecular). To build a molecular model accurately based on the electronic build method that relies on quantum mechanics, the storage capacity and the processor speed should be increased so that it introduced another method (semi-empirical method) to resolve this problem by introducing the experimental spectral values to speed up the calculation calendar style treatment.

Biological methods antibacterial activity

This method involved using a medium (Muller Hinton Agar) that was prepared, poured into a pretty dish, and placed in the autoclave, and then left to cool and solidify so that the medium was ready for the process of the bacteria culture. The bacteria are activated for 24 hours, where they are placed in the pretty dish by cotton swap. This method included making five 6 mm diameter holes by cork borer and equal dimension for each kind of pathogens. The prepared concentration

was added to the holes (0.2 mL) by micropipette per hole with the control hole kept on the DMSO, and then the dishes were incubated in the incubator for 24 hours at 37 °C. The diameter of the zone inhibition was known by the means of a ruler around each hole (16).

Antifungal activity

This method involved using a medium (Potato Dextrose Agar) (PDA) that was prepared, poured into a pretty dish, and placed in the autoclave, and then left to cool and solidify, so that the medium was ready for the process of the fungal culture. The fungal are activated for 72 hours, where the activated fungal are placed in the pretty dish by cotton swap. This method included making five 6 mm diameter holes by cork borer and equal dimension for each kind of pathogens. The prepared concentrations were added to the holes (0.2 mL) by micropipette per hole with the control hole kept on the DMSO, and then the dishes were incubated in the incubator for 72 hours at 28 °C. The diameter of the zone inhibition was known by the means of a ruler around each well (17).

Formation of ligands complexes in solution state

The molar ratio method was used to determine the (M:L) ratio of the complexes by using ethanol absolute by gradually adding the following volumes from the ligand (0.25-5.0 mL) of 10^{-3} M to (1 mL) of 10^{-3} M of each metal ions ($CoCl_2.6H_2O$, $NiCl_2.6H_2O$, $CuCl_2.2H_2O$, $PdCl_2$, $H_2PtCl_6.6H_2O$, and $HAuCl_4.H_2O$) in a volumetric flask 10 ml in size and the absorbance measurements at λ_{max} of the formed complex.

Results and Discussion

The physical properties, metal percentage, and product percentage of ligand and the prepared complexes were listed in Table 1. The elemental analysis shows that the ratio of metal to ligand is 1:1, as summarized in Table 1. The [M= Co(II), Ni(II), Cu(II), Pd(II), Pt(IV), and Au(III)], L= 5-((1 H-indol-1-yl) methylthio)-N-(4-(dimethylamino) benzylidene)-1,3,4-thiadiazol-2-amine. The complexes are air-stable solids, soluble in some solvent such as DMF, DMSO, C_2H_5OH, and CH_3OH, and insoluble in the other common organic solvents.

Table 1: The physical properties of ligand (L) and its complexes prepared in ethyl alcohol solvent

Compound	Color	m.p/°C	Yield %	Atomic Abs.% Cal.(Found)	C	H	N	S
L 393.53	Red	95-97	75	-	61.04 (60.66)	4.87 (3.97)	17.80 (16.90)	16 . 30 (15.56)
Co L 559.37	Brown	255-277	67	10.53 (11.00)	42.94 (43.03)	4.11 (3.47)	12.51 (12.78)	11.46 (10.69)
Ni L 577.12	Light brown	75-77	65	10.16 (10.76)	41.58 (40.98)	4.33 (3.42)	12.12 (11.32)	11.09 (10.91)
Cu L 581.97	Brown	198-200	64	10.91 (10.57)	41.23 (42.11)	4.29 (4.98)	12.02 (11.02)	10.99 (11.08)
Pd L 660.3	Dark Brown	240-242	70	16.11 (15.93)	36.37 (37.15)	3.78 (3.06)	10.59 (11.34)	9.70 (10.04)
Pt L 766.39	Black	Over 360	65	25.45 (26.09)	31.34 (30.77)	3.00 (3.03)	9.13 (8.38)	8.36 (9.26)
Au L 714.84	porphyry	130-132	77	27.55 (27.00)	33.60 (34.44)	2.93 (3.16)	9.80 (8.89)	8.96 (8.00)

Table 2: The electronic spectra, magnetic susceptibility, and conductivity measurement of all prepared compounds

Formula	Absorption (cm^{-1})	Assignment	Conductivity (μ s.cm^{-1})	μeff B.M. Found (Calculated)	Suggested Geometry
L	22935 25250 37038 47393	n → π* n→π* π → π* π → π*	-	-	-
CoL	10235 19841 25641 36101	$^4T_1g \rightarrow {}^4T_2g$ $^4T_1g \rightarrow {}^4A_2g$ $^4T_1g \rightarrow {}^4T_1g(p)$ IL→CoCT	14	3.92 (3.87)	Octahedral
NiL	12196 10206 16000 24814 25974 35460	$^3A_2g \rightarrow {}^1Eg$ $^3A_2g \rightarrow {}^3T_2g$ $^3A_2g \rightarrow {}^3T_1g_{(f)}$ $^3A_2g \rightarrow {}^3T_1g_{(p)}$ IL →NiCT IL →NiCT	18	3.30 (2.82)	Octahedral
CuL	12165 25510	$^2Eg \rightarrow {}^2T_2g$ IL → CuCT	69	1.77 (1.73)	Octahedral
PdL	24570 26525 31152 37313	$^1A_1g \rightarrow {}^1B_1g$ $^1A_1g \rightarrow {}^1Eg$ IL → PdCT IL → PdCT	73	0.00 (0.00)	Square Planer
Pt L	22675 27472 33448 46511	$^1A_1g \rightarrow {}^1T_1g$ $^1A_1g \rightarrow {}^1T_2g$ IL → PtCT IL → PtCT	70	0.00 (0.00)	Octahedral
AuL	23696 28985 32467 43103	$^1A_1g \rightarrow {}^1B_1g$ $^1A_1g \rightarrow {}^1Eg$ IL→ AuCT IL→AuCT	88	0.00 (0.00)	Square Planer

Uv-vis spectra, magnetic susceptibility, and molar conductivity

The UV-vis spectra of the ligand and their metal complexes (Scheme 2) were determined in ethyl alcohol at 25 °C. The electronic spectra data of all prepared compounds are listed in Table 2.

The bands in the region 22935, 25250 and 37038, 47393 cm^{-1} is due to n → π* transition of the non-bonding electrons present on S, N, and to π → π* of aromatic ring in the ligand [18]. The magnetic measurement of brown complex CoL (3.92) B.M indicates that to be paramagnatic and high spin octahedral [19]. The conductivity measurement showed that the complex was nonionic. The electronic spectrum of this complex, Table 2 shows (d-d) transition at (10235, 19841) cm^{-1}, which was assigned to $^4T_1g \rightarrow {}^4T_2g$ and $^4T_1g \rightarrow {}^4A_2g$. Also, bands appeared at (25641, 36101) cm^{-1} which were due to $^4T_1g \rightarrow {}^4T_1g_{(p)}$ and IL → CoCT sequentially [19]. The color light brown of NiL complex appeared bands at 10206, 16000, and 24860 cm^{-1} is assigned to $^3A_2g \rightarrow {}^3T_2g$, $^3A_2g \rightarrow {}^3T_1g_{(f)}$, and $^3A_2g \rightarrow {}^3T_1g_{(p)}$ transition, respectively. Likewise, the forbidden band appeared at 12196 cm^{-1}. Another bands appeared at 25974, 35460 cm^{-1} is attributed IL→ NiCT, respectively, which indicate octahedral geometry of Ni(II). Magnetic moment, 3.30 B.M, showed a higher orbital contribution [19, 20]. The conductivity measurement in DMF appeared that the complex was nonionic [20]. In cupper brown complex, the broadness band in spectrum is attributed to $^2Eg \rightarrow {}^2T_2g$. The magnetic moment for the Cu(II) complex was 1.77 BM. From the conductivity value, it was indicated that the complex was conductive [19, 20] which indicated

the octahedral geometry. The electronic spectrum of Pd(II) complex demonstrated two bands at 24570, 26525 cm^{-1}, which were attributed to $^1A_1g \rightarrow {}^1B_1g$, $^1A_1g \rightarrow {}^1Eg$, and the latter two transitions was due to IL→ PdCT, respectively, of the square planer geometry and another last band was attributed to IL → PdCT transition. The magnetic moment was 0.00 B.M showed that the complexes were of low spin. From the conductivity value, the complex was ionic [21, 22]. When observing the spectrum of the black Pt (IV) complex, four transitions were found. The two transitions bands appeared at the frequency 22675, and 27472 cm^{-1}, which were attributed to $^1A_1g \rightarrow {}^1T_1g$, $^1A_1g \rightarrow {}^1T_2g$ and another two bands were represented IL→PtCT, this transition indicated that the complex was octahedral. The conductivity measurement in DMF appeared that the complex was ionic [21]. In spectrum of AuL the magnetic moment showed that the complex possessed the (porphyry color) and a diamagnetic characteristic and two transitions were appeared in the spectrum of this complex which were attributed to $^1A_1g \rightarrow {}^1B_1g$ and $^1A_1g \rightarrow {}^1Eg$ at 23696, 28985 cm^1, respectively [23]. The conductivity measurement in DMF appeared that the complex was ionic. Also, the bands appeared at 32467, 43103 cm^{-1} were attributed to IL→AuCT, this transition indicated that the complex was a square planer.

Fourier transforms spectroscopy (FT-IR) of ligand and their metal complexes

The FT-IR spectrum for free ligand showed five major bands 1620 cm^{-1}, 1581 cm^{-1}, 1222 cm^{-1}, 740 cm^{-1}, and 2893, 2903 cm^{-1}, returned to ν CH=N_{schiff} (24), νC=$N_{cyclic\ of\ thiadiazole}$ (24), νCSC (18), ν CS (21), and ν (CH_2-N) (25), respectively. Some of these peaks are shifted towards the high or low frequencies when they are coordinated with the metal ions. In all complexes, we observed the stretching vibration peaks of νCH=N_{Schiff}, νC=$N_{cyclic\ of\ thiadiazole}$,νCSC, and νCS. It showed a shift towards at high frequencies except for gold complex in CSC band, it has been shifted towards the lower frequency. This shift indicates the coordination occurrence through the imine group, nitrogen ring of the thiadiazole, and S as tridentate ligand (17). The spectra of all the complexes show the additional medium intensity bands in the range 519-470, 470-412, and 369-320 cm^{-1} assigned to the υ(M-N), υ(M-S), and υ(M-Cl), respectively (18,21). Other bands of the coordinated water and others to water outside the coordinated sphere can be observed in Table 3.

Table 3: The main absorption bands of the infrared spectrum of ligand (L) and its metal complexes

Compound	νC=N_{Schiff}	νC=N_{ring}	νCSC	νCS	νCH2-N	νM-N	νM-S	νM-Cl	Other bands
L	1620	1581	1222	740	2893 2903	-	-	-	
CoL	1651	1600	1230	767	2897 2904	470	439	320	3444 817 767
NiL	1666	1608	1238	758	2893 2903	519	412	343	3309 813 758
CuL	1695	1607	1242	750	2894 2905	513	447	347	3448 3390 821 750
PdL	1647	1589	1238	752	Broad 2904	513	408	369	3387
PtL	1705	1608	1237	755	2894 2906	489	428	345	3444 3394
AuL	1699	1599	1199	760	2891 2906	513	470	331	3441

^{1}H-NMR spectra

^{1}H-MNR spectra of -5((1 H-indol-1-yl) methylthio)-N- (4 -(dimethylamino)benzylidene),1,3,4-thiadiazol-2-amine(L) and its some metal complexes

^{1}H-NMR spectrum of this ligand was recorded in DMSO solvent and shows the following characteristic chemical shifts. In ligand (L), the sharp triplet absorption peak around 5.42, 5.44, and 5.47 was attributed to the CH_2-N proton of methylene group (26). The multiple peaks between 6.68 and 7.68 are due to the aromatic ring of indol and benzene ring (27). A sharp triplet absorption peak around 3.02, 3.02, 3.13 ppm was attributed to proton (N-CH_3) group. Also, the ligand shows signal as peaks at 7.93 and 8.66 ppm attributed to the proton of HC=$N_{thiadiazol}$ and CH=Nimine group (28). In complexes of PtL and AuL, we note that there is a slight shift in azomethane group as a result of its consistency occurrence (Figure 1). Another peaks of ligand, PtL and AuL can be seen in Table 4.

^{13}C-NMR spectra

^{13}C-MNR spectra of -5((1 H-indol-1-yl)methylthio)-N-(4(dimethylamino)benzylidene),1,3,4-thiadiazol-2-amine(L) and its some metal complexes

The spectrum of L shows a signal at 39.73, 40.08 which indicates that the carbon of (CH_3-N) group (29). The signals observed at the range 111.51-131.98 is due to the aromtic ring of indol and benzene ring (29). Another peaks at 63.44 and 164.29 were corresponded to (CH_2–N of methylene group) and (C-S) of 1,3,4 thiadiazole (30), respectively (Figure 2). Another peaks of ligand, PtL and AuL are visible in Table 4.

Solution study

Molar ratio method was used to determine the M: L ratio in ethanol solution suggested that the metal to ligand ratio (1:1) for all complexes which were in agreement with results obtained from solid state, as depicted in Figure 3.

Table 4: Proton and carbon thirteen nuclear magnetic resonance spectra of Schiff-Mannich base ligand and its metal complexes

^{1}H-NMR	^{13}C-NMR
L: ^{1}H-NMR (DMSO-d_6): δ 5.42, 5.44, 5.47 (t, 2H, CH2-N of methylene group), 3.02, 3.04, 3.13 (t, 3H of N-CH_3 group), 6.68-7.68 (m, H-Ar, phenyl ring of indol and benzene ring), 7.93, 8.66 (S, H, HC=N of C=N thiadizol ring and imine group).	L: ^{13}C-NMR (DMSO-d_6): δ 39.73, 40.08 (CH3-N), 63.44 (CH_2-N of methylene group), 154.64 (CH_2-N of imine group), 111.51-131.98 aromtic ring of indol and benzene group), 164.29 (C-S of 1,3,4 thiadiazole.
AuL: ^{1}H-NMR (DMSO-d_6): δ 5.40, 5.41 (d, 2H, CH_2-N of methylene group), 3.42, 3.43, 3.45 (t, 3H, of N-CH_3 group), 6.77-7.42 (m, H-Ar, phenyl ring of indol and benzene ring), 7.66, 8.127.68, 8.44 (S, H, HC=N of C=N thiadizole ring and imine group).	AuL: ^{13}C-NMR (DMSO-d_6): δ 39.80, 40.14 (CH_3-N), 63.44 (CH_2-N of methylene group), 153.64 (CH2-N of imine group), 111.05-131.05 (aromtic ring of indol and benzene group), 165.97 (S-C of 1,3,4 thiadiazole).
PtL: ^{1}H-NMR (DMSO-d_6): δ 5.60, 5.66, 5.67 (t, 2H, CH_2-N of methylene group), 3.02, 3.40, 3.41 (t, 3H, of N-CH_3 group), 6.77-7.34 (m, H-Ar, phenyl ring of indol and benzene ring), 7.68, 8.44 (S, H, HC=N of C=N thiadizol ring and imine group).	PtL: ^{13}C-NMR (DMSO-d_6): δ 39.88, 40.04 (CH_3-N), 66.44 (CH_2-N of methylene group), 156.61 (CH_2-N of imine group), 112.51-131.98 aromtic ring of indol and benzene group), 169.29 (S-C of 1,3,4 thiadiazole).

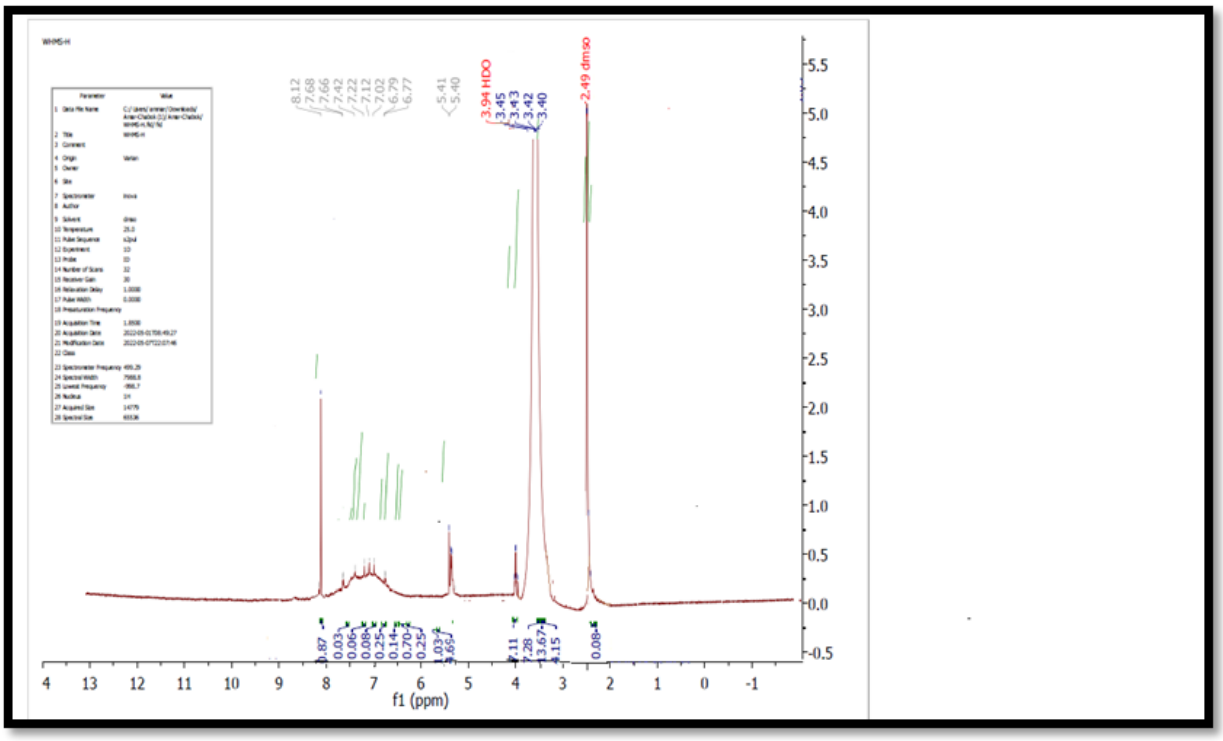


Figure 1: ^{1}H-NMR spectrum of AuL

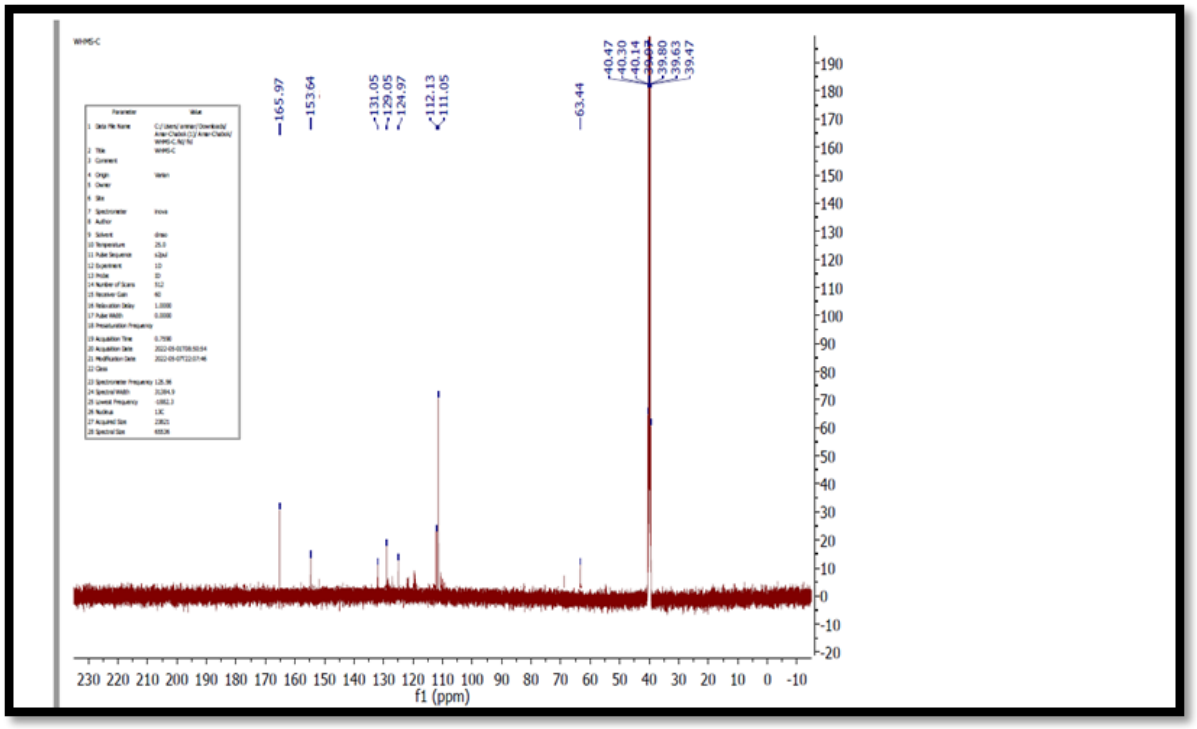


Figure 2: ^{13}C-NMR spectrum of AuL

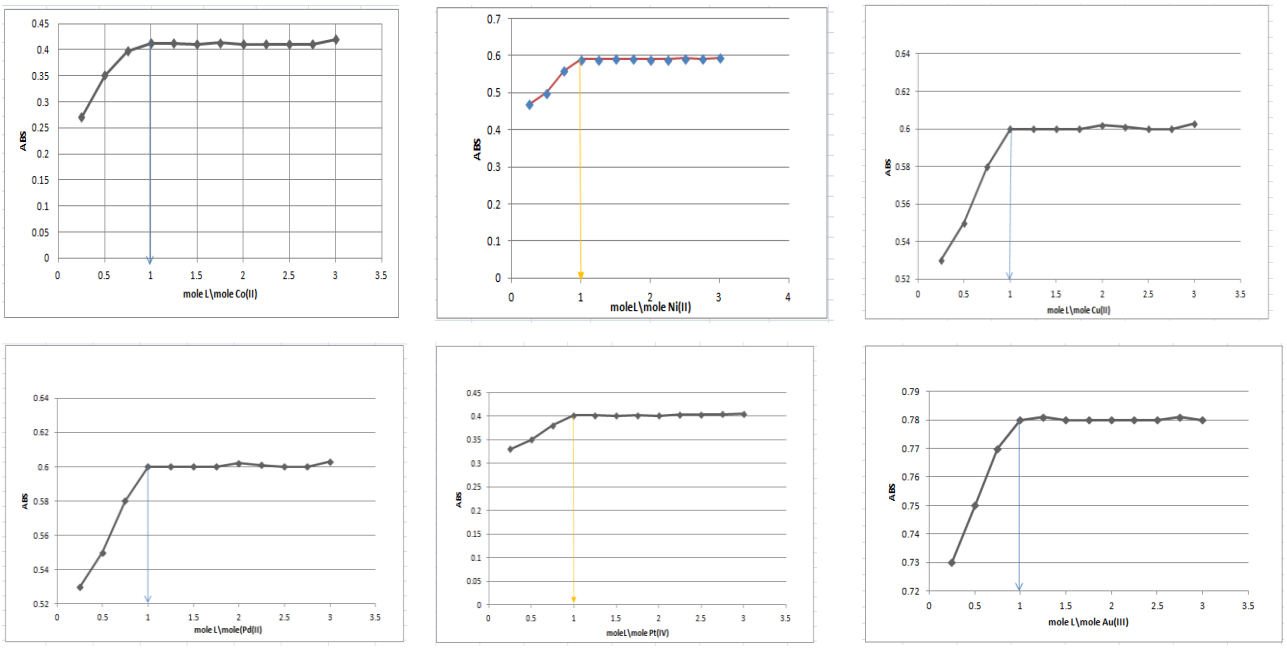


Figure 3: The M:L chart of all prepared complexes

Table 5: Heat of formation, binding energy (in KJ.mol^{-1}) and dipole moment (in Debye) for ligand S_2, L, and its metal complexes by using Hyper Chem 8.0.7 program

	PM3			ZINDO/1			AMBER	
Compound	$\Delta H°_f$	ΔE_b	μ	$\Delta H°_f$	ΔE_b	μ	$\Delta H°_f = \Delta E_b$	μ
S2	656.4017158	-6242.1693	2.85	-7715.4465	-5134.2285	3.13		
L	181.3194910	-4924.2185	6.91	-6635.5654	-82479.5643	3.63		
CoL	-212.9164	-7812.4671	1.67	-23460.3895	-33921.2417	3.93		
NiL	-210.6189	-6150.9070	2.53	-30721.8766	-72009.2286	5.81		
CuL	-519.4129	-8413.7021	4.82	-79810.3316	-9876.8290	3.32		
PdL	-	-		-	-	7.90	178.3453	0
PtL	-	-		-	-	3.90	305.3632	0
AuL							180.2750	0

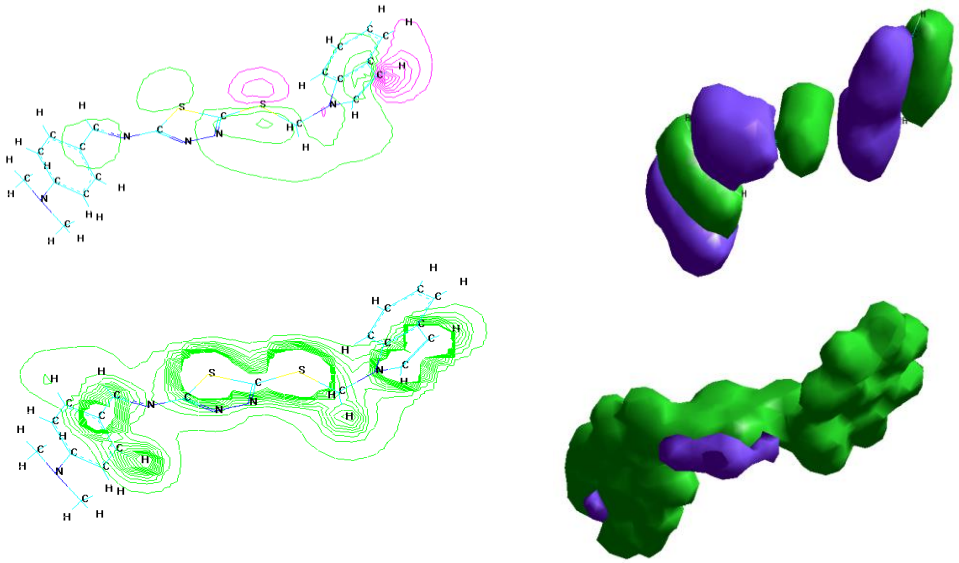


Figure 4: HOMO, LUMO, and electrostatic potential in 2D and 3D for ligand (Schiff-Mannich) base by using Hyper chem 8.0.7 program

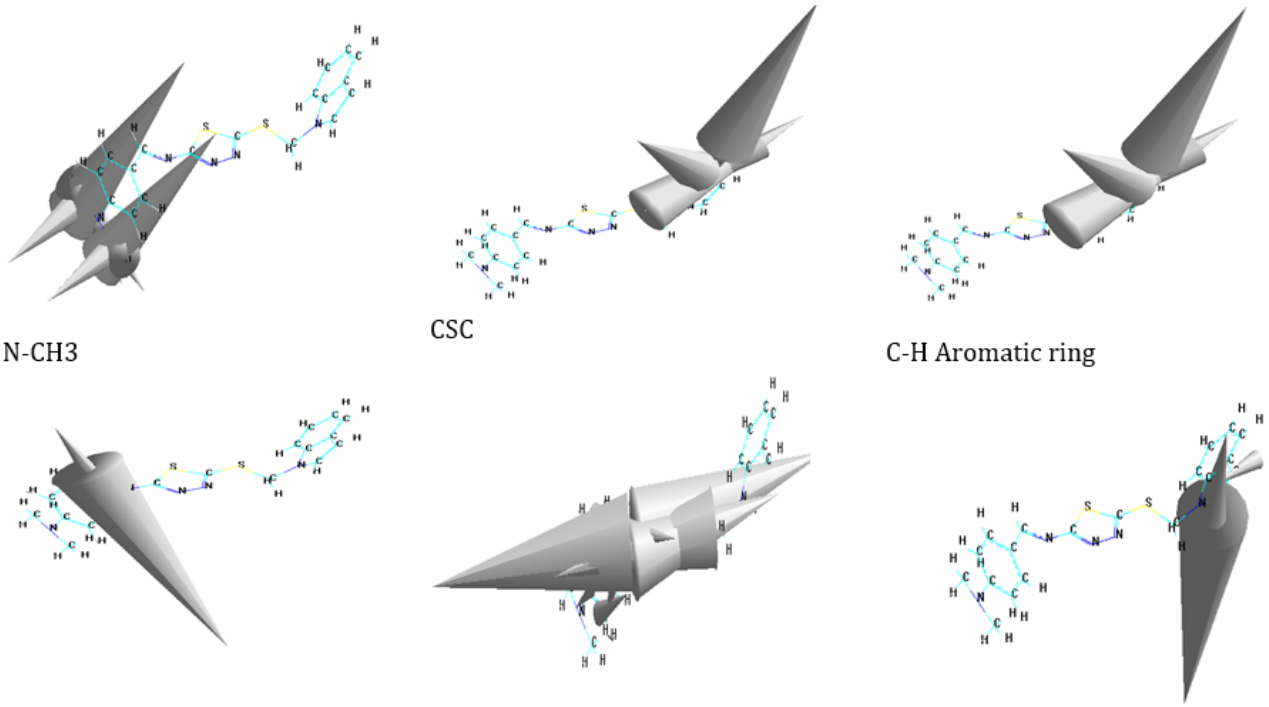
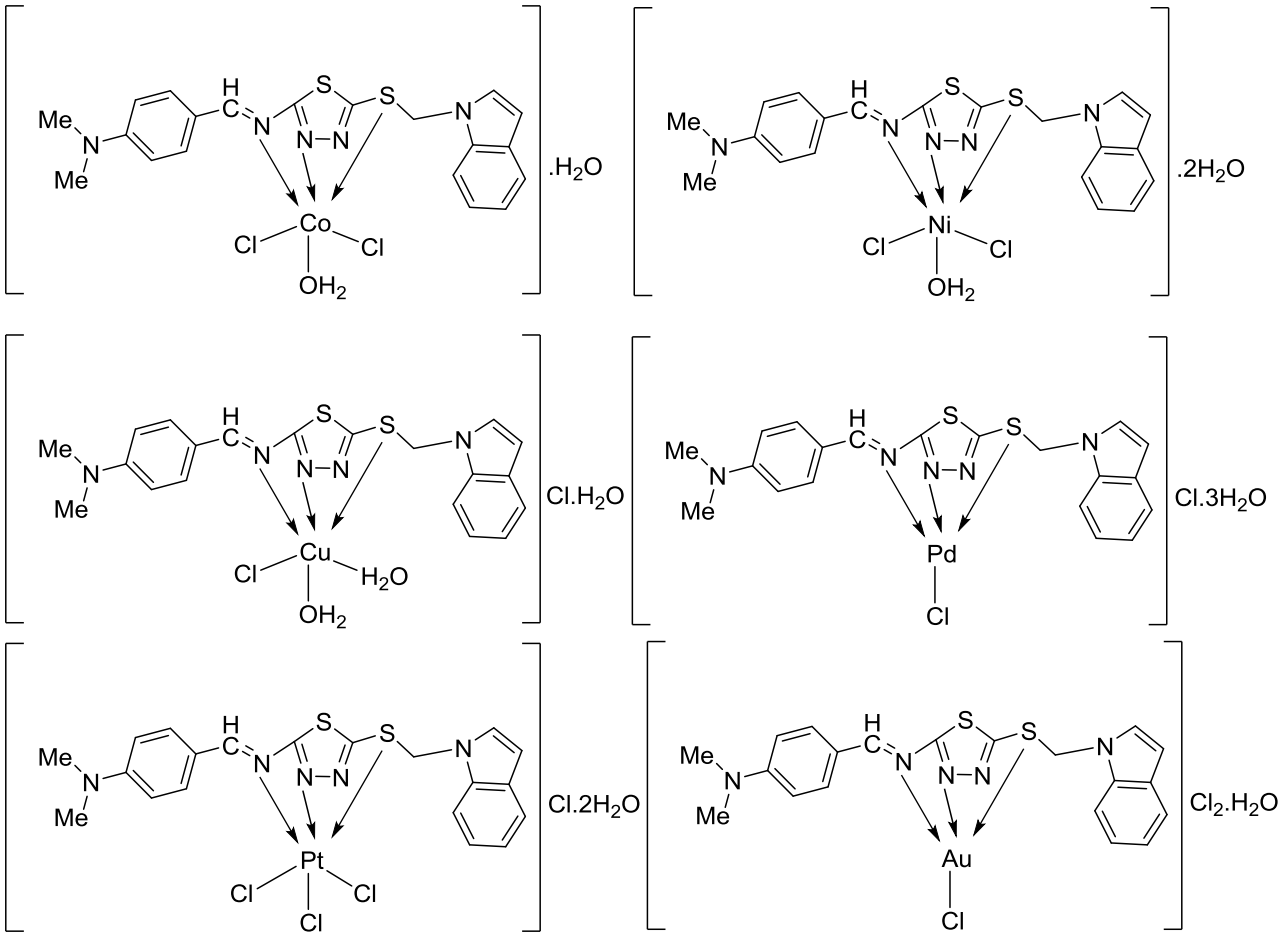


Figure 5: Vibration frequency of some functional groups of L by using Hyper chem 8.0.7 program



Scheme 2: The suggested geometry of all prepared complexes

Biological activity

The antibacterial and antifungal activity of ligand and the prepared complexes was measured at a concentration of 0.02 M and two types of gram-positive and gram-positive bacteria were used. The gram-negative bacteria *Klebsiella* and *E.Coli* and gram-positive bacteria *staphylococcus and Bacillus* as well as fungi *Candida.* Amoxicillin was used as an antibacterial drug and metronidazole as an antifungal drug to compare the effectiveness of the prepared compounds with the drug.

Theoretical study

Hyperchem 8.0.7 program was used to calculate the (ΔHf^0) and (ΔE^0) of L and all complexes. Table 5. HOMO and LUMO of L was calculated Figure 4. The vibration frequencies of the ligand were calculated and the experimental results were compared with the theoretical results, and the error ratio between the two methods was calculated Figure 5 and Table 6.

The obtained results proved that all the prepared compounds which represent the ligand and the prepared complexes, have a higher activity than the used drug, in addition to that some of the prepared complexes have an excellent activity against a specific type of bacteria. As the cobalt complex possesses high activity against *Staphylococcus aureus* and *E.coli*, while palladium and platinum complexes possess high efficacy towards *Klebsiella*.

Table 6: Antibacterial activity of L and its metal complexes at 0.02 M

Inhibition Zone (mm.)						
Compounds		Gram-positive		Gram-negative		Fungi
		staph	*Bacillus*	*E.coli*	*klebsiella*	*Candida*
1	COL	27	18	27	20	45
2	NiL	17	15	13	13	35
3	CuL	17	16	17	15	45
4	PdL	10	18	12	31	45
5	PtL	20	25	15	30	40
6	AuL	12	13	12	13	20
7	DMSO	-ve	-ve	-ve	-ve	-ve
8	L	15	18	9	13	25
9	Amoxicillin	9	12	8	9	-
10	Metronidazole					17

Conclusion

The ligand 5((1 H -indol-1-yl) methylthio)-N- (4-(dimethylamino)benzylidene),1,3,4-thiadiazol-2-amine (L) has been successfully synthesized. A number of techniques have been used to characterize the prepared complexes. The proposed geometric structure of the complexes was diagnosed as the octahedral was proposed for Co(II), Ni(II), Cu(II), Pt(IV), and square planer geometry for the Pd(II) and Au(III). The metal to ligand ratio was calculated in the solution, and the result proved consistent with the solid state. The biological activity of all prepared compounds was studied at 0.02 M, all the prepared complexes proved highly effective in inhibiting the selected types of positive and negative bacteria and *Candida* fungi. The increased effectiveness of the complexes can be attributed to the overtone's concept and Tweedy's theory. The ligand and the complexes prepared theoretically were also studies by using Hyper chem-8.0.7 program in calculating the heat of formation and binding energy. The study proved that the complexes are more stable than the ligand. Also, the vibration frequencies in FT-IR spectrum of ligand were theoretically calculated and compared with the experimental data and the error ratio was calculated between the two methods.

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Authors' contributions

All authors contributed to data analysis, drafting, and revising of the paper and agreed to be responsible for all the aspects of this work.

Conflict of Interest

The author declared that they have no conflict of interest.

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