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Design, Biological and Theoretical Study of New Mixed Ligands Complexes of Schiff Base Derived from Sulfabenzamide and 1,10-phenanthroline

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Abstract

A new Schiff base ligand was prepared via a condensation reaction. The synthesis involved combining N-(4-aminophenylsulfonyl) benzamide (also known as sulfabenzamide) with indoline-2,3-dione. To facilitate the reaction, three drops of glacial acetic acid were added. This process yielded the ligand N-(4-(2-oxoindoline-3-ylideneamino) phenylsulfonyl) benzamide, designated as (L). Mixed ligand complexes were prepared in a molar ratio (1:1:1) (M:1,10-phen, L) at concentrations of 10^{-4}M by interacting L and 1,10-phenanthroline, with the following metal ions (Cr^{+3}, Mn^{+2}, Zn^{+2}, Pd^{+2}, Cd^{+2}, Pt^{+4}). These complexes exhibited different geometric shapes, including (octahedral for both Cr^{+3}, Mn^{+2}, Pt^{+4}, tetrahedral for Zn^{+2} and Cd^{+2}, and square planar for Pd^{+2}) . These prepared complexes were characterized by several techniques such as C.H.N.S, FT-IR, molar conductivity, UV-Vis spectra, magnetic susceptibility and atomic absorption. The ligands were characterized by FT-IR, UV-visible,^{1}H-NMR, ^{13}C-NMR, C. H. N. S and mass spectra. The results showed that the ligand (L) behaves as a bidentate chelating ligand that binds to metal ions through donor N, and O atoms. The biological activity of ligand (L,1,10-phen) and mixed ligands complexes was evaluated against two types of bacteria (positive and negative) and one type of fungi at a concentration of 0.02M. The results demonstrated that the prepared complexes have high inhibition of all types of bacteria and fungi compared to the standard drug and the ligand (1,10-phen). The standard heat of formation and binding energy for ligand (L) and all complexes produced were calculated using the Hyper-Chem8.0.7 program. Additionally, the vibration frequencies as well as the HOMO and LUMO were studied for the ligand alone. When comparing the practical and theoretical vibration frequencies of the ligand, it was found that the results of the theoretical study and experimental were close in result to the error rate within the permissible range.

Keywords: Schiff base, mixed ligands complex, Biological and Theoretical study, sulfabenzamide

تصميم ودراسة بيولوجية ونظرية لمعقدات ليكاندات مختلطة جديدة من قاعدة شف المشتقة من السلفابنزاميد و 1،10-فينانثرولين

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الخلاصة

تم تحضير قاعدة شف الجديدة من خلال تفاعل التكثيف. يتضمن التحضير الجمع بين بنزاميد N-(4-أمينوفينيل سلفونيل) (المعروف أيضًا باسم سلفابنزاميد) مع إندولين-2،3-دايون. لتسهيل التفاعل ، تمت إضافة ثلاث قطرات من حامض الخليك الثلجي. أنتجت هذه العملية المركب N-(4-(2-oxoindoline-3-ylideneamino)phenylsulfonyl)benzamide ، والمسمى بـ (L) . تم تحضير معقدات الليكاند مختلطة بنسبة مولية (1:1:1) (M:1,10-phen,L) بتركيز 10^{-4} مولاري عن طريق تفاعل الليكاند L و 1و10-فينانثرولين مع الايونات الفلزية التالية $(Cr^{+3},Mn^{+2},Zn^{+2},Pd^{+2},Cd^{+2},Pt^{+4})$. أظهرت هذه المعقدات اشكال هندسية مختلفة منها ثماني السطوح لكل من معقد Cr^{+3} وMn^{+2} وPt^{+} ورباعي السطوح Zn^{+2} وCd^{+2} ومربع مستوي لمعقد Pd^{+2} . تم تشخيص هذه المعقدات المحضرة بعدة تقنيات مثل C.H.N.S ، FTIR ، الموصلية المولارية ، الاشعة فوق البنفسجية – المرئية والحساسية المغناطيسية والامتصاص الذري. شخصت الليكاندات بطيف الأشعة تحت الحمراء والأشعة فوق البنفسجية – المرئية وطيف الرنين النووي المغناطيسي للبروتون والكاربون وطيف الماس. اظهرت النتائج ان الليكاند (L) يتصرف كـ ليكاند مخلبي ثنائي السن يرتبط بأيونات الفلزات من خلال ذرات N,O المانحة. تم اجراء الفعالية البايولوجية لليكاند (L,1,10-phen) ومعقدات الليكاندات المختلطة وقد قيمت باستخدام نوعين من البكتريا (الموجبة والسالبة) ونوع واحد من الفطريات عند تركيز 0.02 مولارية . أظهرت النتائج ان المعقدات تمتلك فعالية تثبيط عالية ضد كل أنواع البكتريا والفطريات المستخدمة مقارنة مع الدواء القياسي و 1،10-فينانثرولين . تم حساب حرارة التكوين القياسية وطاقة الترابط لليكاند (L) وجميع المعقدات المحضرة باستخدام برنامج الـ Hyper chem8.07 . إضافة الى دراسة ترددات الاهتزاز كذلك الهومو واللومو لليكاند فقط . عند مقارنة ترددات الاهتزازات العملية والنظرية لليكاند وجد حدوث تقارب كبير بينهما مع وجود نسبة خطأ ضمن المدى المسموح.

1. Introduction

Chemists and researchers who have achieved therapeutic success in treating severe diseases and the enhancement of various medications find coordination chemistry to be a compelling area of study [1]. Sulfabenzamide is used as an antimicrobial drug and contains a crucial functional group. By modifying this group in combination with sulfonamides, a diverse array of drugs can be developed with anti-diabetic, antibacterial, and anti-tumor properties. Sulfabenzamide contains N, O, and S donor atoms in various positions, enabling it to function as multi-chelated ligands, they can chelate with different structural types and different metal ions, and the drug activation of these derivatives is often improved through coordination with metal ions [2]. Schiff-bases a distinctive class of ligands characterized by a variety of donor atoms that show amazing coordination patterns with transition metals. The presence of an azomethine linkage significantly influences biological activity. A considerable number of Schiff bases derived from different amines have been investigated using diverse techniques and have proven to have intriguing uses in materials chemistry, catalysis, and industry[3]. The most widely used class of organic molecules are Schiff bases, which are significant organic compounds. The advancement of science has been greatly facilitated by compounds with double-bond carbon-nitrogen functional groups in their molecules, particularly in medicinal chemistry. The azomethine group's versatility and ease of formation make them helpful in day-to-day living [4]. Because of their amazing chemical characteristics and wide range of applications, Schiff bases and their metal complexes have been extensively studied and have proven to be attractive leads for both synthetic and structural study due to their comparatively simple synthesis and structural variety [5]. Numerous biological actions, including antibacterial, antifungal, antidiabetic, antitumor, antiproliferative, anticancer, anticorrosive, and anti-inflammatory properties, have been demonstrated for Schiff bases with imino functionality [6]. Recently, there has been significant interest among young scientists in exploring the transition metal complexes of Schiff base ligands because of the wide range of ligand structures that can be achieved based on the specific industrial or biological applications of the ketones or amines that are employed [7]. The antibacterial and antimicrobial properties of sulfabenzamide are well established. Water was previously employed as an anti-solvent and carbon dioxide was used to crystallize the sulfabenzamide molecule [8, 9] Sulfabenzamide-Schiff bases are some important classes of these compounds. However, the metal complexes of sulfabenzamide (SBZ) have not been individually studied. Therefore, this paper discusses the synthesis of metal complexes of sulfenzamide and the evaluation of their antibacterial and antifungal activities.

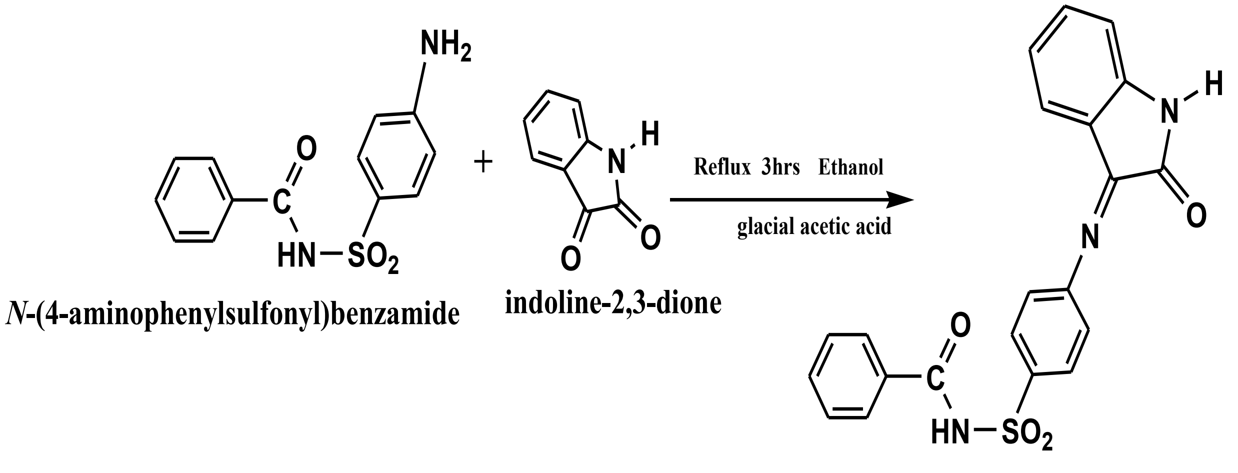
2. Experimental

2.1. Materials and Methods

In this study, chemicals of the highest purity were utilized. The C.H.N.S elemental data were analysed using an Eager 300 elemental analyzer. Magnetic susceptibility measurements using a Mode (Magnetic Susceptibility Balance MSB-MKI) device. Molar conductivity was measured using a WTW device at a temperature of 25°C, and $1*10^{-3}$M, DMF was used as a solvent. FT-IR spectra were measured using Shimadzu Corporation 8400 Fourier Infrared Transform Spectrophotometer, covering a wave number range of 4000-400cm^{-1} and 4000-200cm-1 in KBr and CsI respectively. The UV-visible absorption spectra were obtained in DMSO solution using a UV-visible (UV-1800) Shimadzu Spectrophotometer. Using a Shimazu atomic absorption 670 Flam spectrophotometer, metal contents were measured. The ^{1}HNMR and ^{13}C NMR spectra were acquired using the Brucker (400MHz) Spectrometer. The Schiff base ligand (L) was measured using a GC-MS (Gas chromatography Spectrometry) device, specifically the Agilent GC7890A model. The melting point of all prepared compounds was measured by a type device Gallen Kamp M.F.B-60

2.2. Synthesis of Schiff base ligand N-(4-(2-oxoindoline-3-ylideneamino) phenylsulfonyl)benzamide (L)

In a round bottom flask, 0.27 g (0.001 mol) of sulfabenzamide was dissolved in a mixture of 10 mL of absolute ethanol and two drops of DMF in the presence of heat 60^{0}C, then (0.14 g, 0.001mol) of isatin dissolved in (15 ml) of absolute ethanol. The two solutions were then combined, and three drops of glacial acetic acid after that for 3 hours at a temperature of 80^{0} C was refluxed [10]. After refluxing, the product was cooled at room temperature to obtain orange crystals and it was recrystallized using ethanol solvent, as shown in Scheme 1. The yield was 80%, with a melting point range of 138-140°C.



Scheme 1: synthesis of Schiff base ligand N-(4-(2-oxoindoline-3-ylideneamino) phenylsulfonyl)benzamide (L)

2.3. Preparation of new complexes from Schiff base ligand (L)

The complexes were synthesised in ethanol by reacting 1 mmol of various metal ions with different valences: 0.26g $CrCl_3.6H_2O$, 0.19g $MnCl_2.4H_2O$, 0.13g $ZnCl_2$, 0.17g $PdCl_2$, 0.20g $CdCl_2.H_2O$ and 0.12g $H_2PtCl_6.6H_2O$, along with 0.1 g of Schiff base ligand and (0.1g 1,10-phenanthroline) in a molar ratio of(1:1:1) and refluxing for 3 hours. Different coloured precipitates were obtained. The precipitate was then filtered and rinsed several times with ethanol. Its weight was recorded, and the percentage yield was calculated as shown in Table 1

2.4. Antibacterial and antifungal activity

The biological activity was assessed using the well diffusion method. Mueller Hinton agar was used for bacterial cultures, and potato dextrose agar was used for fungal cultures. The prepared samples were finely ground and dissolved in a DMSO solution at a concentration of 0.02M for each sample. These solutions were then evenly spread across the entire surface of the agar medium. Wells of 6 mm diameter were made in the agar using a sterile borer. The wells were filled with 100 microliters of the solutions to be tested. Each agar plate contained a single bacterial or fungal isolate. This process was repeated for all prepared solutions and each bacterial and fungal isolate. The plates were incubated under appropriate conditions for bacterial and fungal growth. The diameter of the inhibition zones around the wells was measured to determine the antibacterial and antifungal activity of the solutions. Bacterial plates were incubated at 37 ^{0}C degrees for 24 hours. As for the fungi dishes, they were incubated for 72 hours at a temperature of 28 ^{0}C. The activity was read by observing the diameter of inhibition around the holes loaded with solutions and measuring it in mm using a transparent acrylic ruler [11,12].

3. Results and discussion

3.1 Physicochemical Feature:

A new orange-coloured Schiff base ligand (L), along with 1, 10-phen and all mixed ligands complexes are soluble in ethanol, methanol, DMF and DMSO. The measurable physical and analytical results are presented in Table 1. It was found that the calculated data and elemental analysis results were in good agreement, confirming a metal-to-ligands ratio (L: M: L) as (1:1:1) for valence measured.

Table 1: Some physical properties of two ligands and six mixed ligand complexes

Symbol and Formula/M.wt	Colour	m.p/^{0}C	Yield %	Molar ratio (M:L)	Atomic Abs(%)Cal (Found)	Elemental analysis Calc.(Found)				
						C%	H%	N%	O%	S%
1,10-phen 180.21	White	292-294	-	-	-	79.90 (80.11)	4.43 (3.76)	15.53 (16.17)	-	-
Ligand(L) 405.08	Orange	120-140	73	-	-	62.20 (63.11)	3.70 (4.09)	10.36 (11.18)	15.79 (16.59)	7.92 (8.34)
[Cr(L)1,10-phen Cl_2]Cl 744.549	Dark brown	162-164	70	(1:1:1)	6.98 (7.09)	53.25 (54.00)	3.09 (2.51)	9.41 (10.30)	8.60 (9.47)	4.31 (5.11)
[Mn(L)1,10-phen Cl_2] 711.134	Pale orange	250decompose	70	(1:1:1)	7.72 (8.34)	55.68 (56.12)	3.23 (4.17)	9.84 (10.29)	8.99 (9.67)	4.50 (5.12)
[Zn(L)1,10-phen]Cl_2 721.576	Light orange	198-200	82	(1:1:1)	9.06 (10.06)	54.88 (55.45)	3.18 (3.01)	9.70 (10.28)	8.86 (9.56)	4.44 (5.37)
[Pd(L)1,10-phen]Cl_2 762.616	Light brown	80-82	67	(1:1:1)	13.95 (14.78)	51.92 (52.34)	3.01 (3.89)	9.17 (9.67)	8.39 (9.18)	4.20 (5.18)
[Cd(L)1,10-phen]Cl_2 768.607	Dark orange	118-120	85	(1:1:1)	14.62 (13.20)	51.52 (52.11)	2.99 (3.17)	9.10 (10.02)	8.32 (9.27)	4.17 (5.07)
[Pt(L)1,10-phen Cl_2]Cl_2 922.192	Brown	128-130	64	(1:1:1)	21.15 (21.64)	42.94 (43.23)	2.49 (3.34)	7.59 (8.17)	6.93 (7.09)	3.48 (4.10)

L=ligand, 1,10-phen= 1,10-phenanthroline

3.2. Molar ratios

The ratio of the metal to the ligand was determined using the molar ratio method, with both the metal and ligand at a concentration of $1x10^{-3}$. Various volumes of the ligand, ranging from 0.25 ml to 3 ml, were used while keeping the volume of the metal constant at 1 ml. The study proved that the ratio of the ligand to the metal ion is a ratio of 1:1:1. Figure 1 graphically shows the relationship between the absorbance at the wavelength of the highest absorption and the molar ratio L\M.

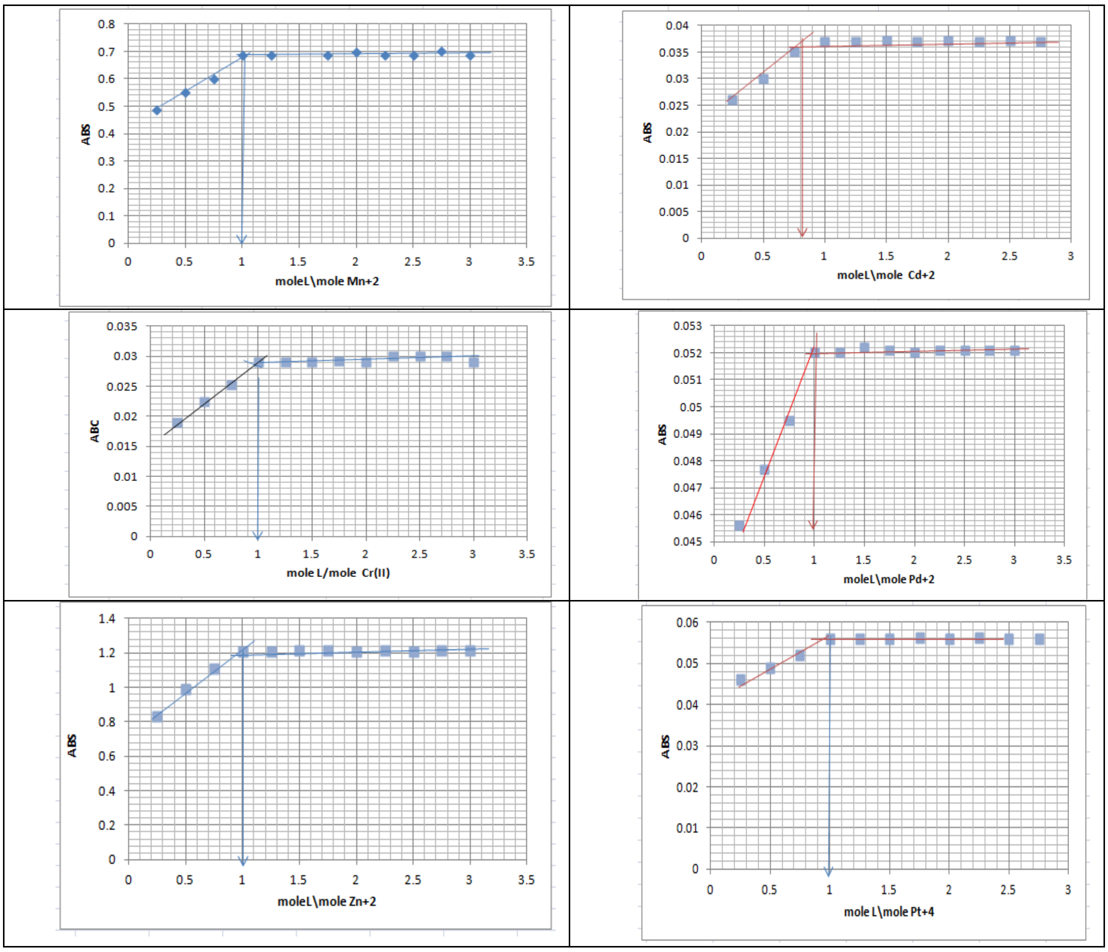


Figure 1: Molar ratios of complexes

3.3 UV-Vis spectra, conductivity and magnetic moment.

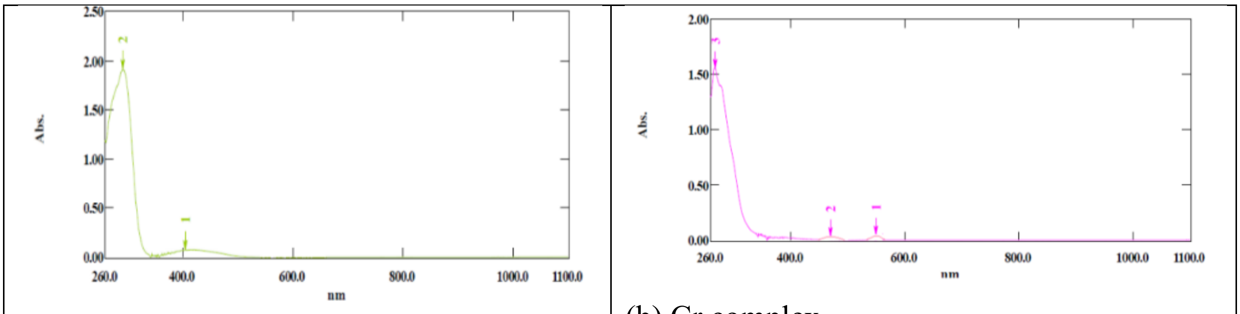
The UV-visible spectra of the Schiff base ligand L, 1,10-phenanthroline, and all mixed ligand complexes were determined using DMSO as a solvent at 25 °C, with a concentration of$1x10^{-3}$. The solution was then diluted until the desired transition was obtained. The spectra result for all the prepared compounds are shown in Table 2. The ligand(L) frequency bands in the region 24752 and 34246cm^{-1} are due to the $n\rightarrow\pi^*$ transition of the nonbonding electron and $\pi\rightarrow\pi^*$ due to the aromatic ring electron transition [13]. The spectrum of dark brown chromium mixed ligand complex [Cr(L)1,10-phen Cl_2]Cl complex shows that the transitions (572 nm, 17482cm^{-1}), (492 nm, 20325cm^{-1}) and (268 nm,37313cm^{-1}) which attributed to $^4A_2g\rightarrow{}^4T_2g$, $^4A_2g\rightarrow{}^4T_1g_{(f)}$ and $^4A_2g\rightarrow{}^4T_1g_{(p)}$, from magnetic experimental data and conductivity measurement the result show that complex is octahedral geometry and good ionic properties [14,15]. In the orange complex [Mn(L)1,10-phen Cl_2] there were seven absorption peaks, the peaks at (825 nm,12121cm^{-1}),(740 nm,13513cm^{-1}) and (632nm,15822cm^{-1}) assigned to the $^6A_1g\rightarrow{}^4T_1g_{(G)}$,$^6A_1g\rightarrow{}^4T_2g_{(G)}$, $^6A_1g\rightarrow{}^4A_1g$, $Eg_{(G)}$

respectively, and four peaks appeared at (405nm,24691cm^{-1}),(361nm,27700cm^{-1}) and (302nm, 331122 cm^{-1}) and (235nm, 42553cm^{-1}) which are attributed to charge transfer, $n\rightarrow\pi^*$ and $\pi\rightarrow\pi^*$ respectively. Measurement of its conductivity at 23 $\mu s.cm^{-1}$ also the magnetic moment showed that the complex is non-ionic and octahedral geometry [16]. The electronic spectrum of light orange zinc $[Zn(L)1,10\text{-}phen]Cl_2$ the absorption bands at (408nm,24509 cm^{-1}) has been assigned to charge transfer Zn→LCT and (269nm,37174cm^{-1}) due to $\pi\rightarrow\pi^*$ Figure 5. Conductivity measurements 152 $\mu s.cm^{-1}$ found that the complex is ionic from UV-vis, and magnetic moment and confirmed that the complex has tetrahedral geometry [17,18]. In the spectrum of the Light brown $[Pd(L)1,10\text{-}phen]Cl_2$ complex the bands appear at (478nm, 20080cm^{-1}) and (422nm, 23696 cm^{-1}) which are attributed to $^1A_1g\rightarrow{}^1B_1g$ and $^1A_1g\rightarrow{}^1Eg$ and a peak at (265nm,37735cm^{-1}) which belongs to transition $\pi\rightarrow\pi^*$. Measurement of its conductivity at 136 $\mu s.cm^{-1}$ also showed that the complex is ionic and electrolytic the magnetic moment indicates that the low spin complex [19]. The spectrum of dark orange $[Cd(L)1,10\text{-}phen]Cl_2$ complex exhibited peaks of (426nm,23474cm^{-1}) ascribed to the Cd→LCT and (289nm,34602cm^{-1}),(278nm,35971cm^{-1}) and (267nm,37453cm^{-1}) are associated to the transitions $\pi\rightarrow\pi^*$ respectively. The conductivity measurement of complex 148 $\mu s.cm^{-1}$ appeared that be ionic, zero magnetic moment confirms that the complex has a tetrahedral shape [20,21]. When observing the spectrum brown of $[Pt(L)1,10\text{-}phen\ Cl_2]Cl_2$ complex, five transitions were found. The forbidden transitions band appeared at the frequency (906nm,11037cm^{-1}) which was attributed to $^1A_1g\rightarrow{}^3T_1g$ and another two bands appeared at (561nm, 17825cm^{-1}), (402nm, 24813cm^{-1}) belonging to $^1A_1g\rightarrow{}^1T_1g$, $^1A_1g\rightarrow{}^1T_2g$ other two bands represented $\pi\rightarrow\pi^*$. Conductivity measurement showed that the complex is ionic Figure 2 [22, 23].

Table 2: The electronic transition DMF solvent, assignment, μeff in B.M and conductivity

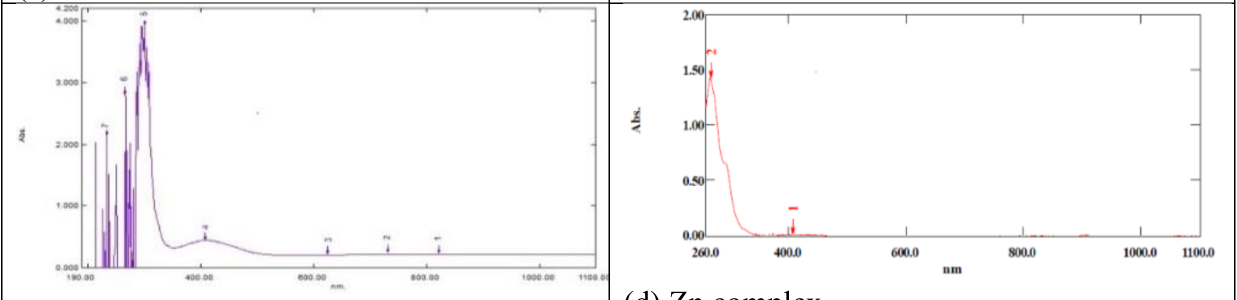
Formula	λ nm	υcm^{-1}	Assignment	Suggested Geometry	μeff B.M.Found(Calculated)	Conductivity $\mu s.cm^{-1}$
Ligand(L)	404 292	24752 34246	$n\rightarrow\pi^*$ $\pi\rightarrow\pi$	--	--	--
1,10-phen	328 266	30487 37593	$n\rightarrow\pi^*$ $\pi\rightarrow\pi^*$			
$[Cr(L)1,10\text{-}phen\ Cl_2]Cl$	572 492 268	17482 20325 37313	$^4A_2g\rightarrow{}^4T_2g$ $^4A_2g\rightarrow{}^4T_1g_{(f)}$ $^4A_2g\rightarrow{}^4T_1g_{(p)}$	Oh	3.36 (3.87)	73
$[Mn(L)1,10\text{-}phen\ Cl_2]$	825 740 632 405 361 302 235	12121 13513 15822 24691 27700 33112 42553	$^6A_1g\rightarrow{}^4T_1g_{(G)}$ $^6A_1g\rightarrow{}^4T_2g_{(G)}$ $^6A_1g\rightarrow{}^4A_1g$, $Eg_{(G)}$ $n\rightarrow\pi^*$ $n\rightarrow\pi^*$ $n\rightarrow\pi^*$ $\pi\rightarrow\pi^*$	Oh	4.89 (5.91)	23
$[Zn(L)1,10\text{-}phen]Cl_2$	408 269	24509 37174	ZnL→CT $\pi\rightarrow\pi^*$	T.H.	0.00 (0.00)	152
$[Pd(L)1,10\text{-}phen]Cl_2$	478 422 265	20080 23696 37735	$^1A_1g\rightarrow{}^1B_1g$ $^1A_1g\rightarrow{}^1Eg$ $\pi\rightarrow\pi^*$	Sq	0.00 (0.00)	136
$[Cd(L)1,10\text{-}phen]Cl_2$	426 289	23474 34602	Cd → L CT $\pi\rightarrow\pi^*$	T.H.	0.00 (0.00)	148

	278 267	35971 37453	$\pi\rightarrow\pi^*$ $\pi\rightarrow\pi^*$			
[Pt(L)1,10-phen Cl_2]Cl_2	906 561 402 299 270	11037 17825 24813 33444 37037	$^1A_1g\rightarrow{}^3T_1g$ $^1A_1g\rightarrow{}^1T_1g$ $^1A_1g\rightarrow{}^1T_2g$ $\pi\rightarrow\pi^*$ $\pi\rightarrow\pi^*$	Oh	0.00 (0.00)	159



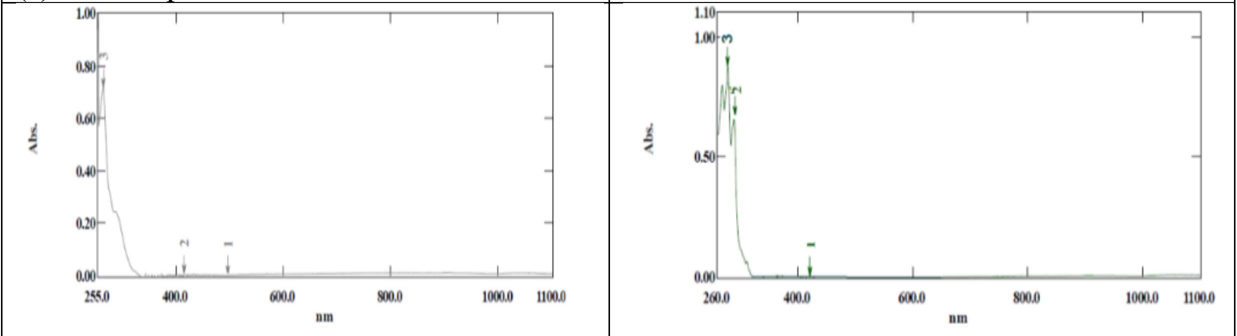
(a) L

(b) Cr complex



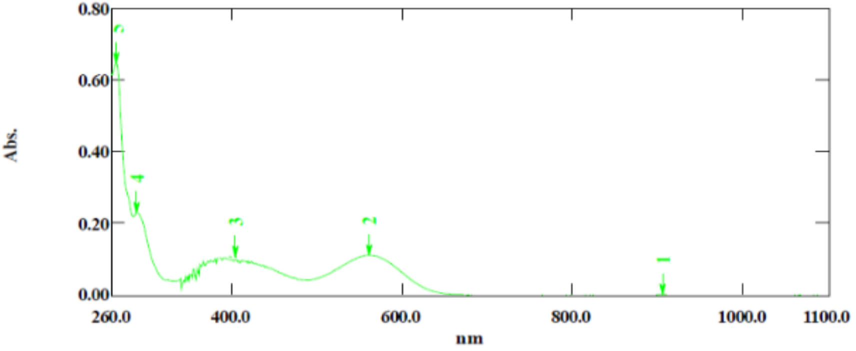
(c) Mn complex

(d) Zn complex



(f) Pd complex

(g) Cd complex



(h) Pt complex

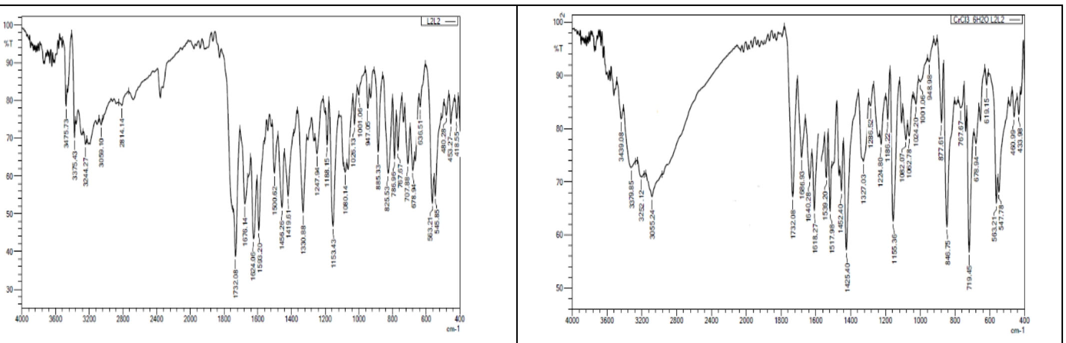
Figure 2: UV-Vis spectra for L and Complexes

3.4. Fourier transform infrared spectra of Schiff base Ligand,1,10-phenanthroline and all mixed ligands complexes

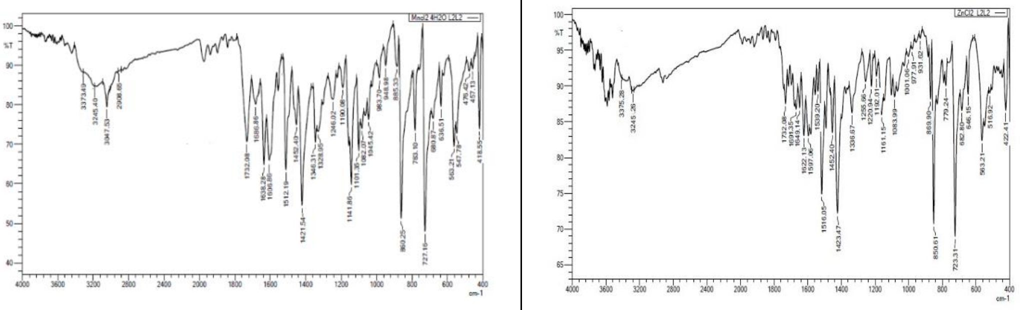
All ligands and mixed ligands complexes were measured using Fourier transform infrared spectroscopy spectra. The spectra of the bands of (L and 1,10-phen) showed the active group, including (vC=O, vC=O$_{istain}$, vC=N, vNH, vNH$_{(istain)}$) Table 3, Figure 3 which shows the frequencies 1732, 1676, 1624, 3244,3375 cm^{-1} when bands are coordinated with a metal ion, all the coordinated bands shifted to higher frequencies (vC=O$_{istain}$, vC=N ,vC=N$_{1,10\text{-}phen}$)[24,25]. The above results show that the Schiff base ligand has a bidentate from behavior through its coordination with the oxygen and nitrogen atoms that belong to the C=O group and imine group, which coordinates with a metal ion (Cr^{+3}, Mn^{+2}, Zn^{+2}, Pd^{+2}, Cd^{+2}, Pt^{+4}), Figure 4. Some of the prepared complexes exhibited bonding, while the frequencies of other vC=O and vNH groups remained unchanged, indicating that there were no coordinated through these groups. The (C=N$_{1,10\text{-}phen}$) also coordinated through to nitrogen atoms when the bands were shifted from (1606 to 1622)cm^{-1}. In addition, new bands appeared that belong to the (vM-O), (vM-N) and (vM-Cl) in range (553- 563) cm^{-1}, (460-480) cm^{-1}, (329-391)cm^{-1} respectively, these bands confirm the consistency of the identified groups [26, 27].

Table 3: Vibration frequencies of important active groups in ligands and mixed ligands complexes by infrared spectroscopy

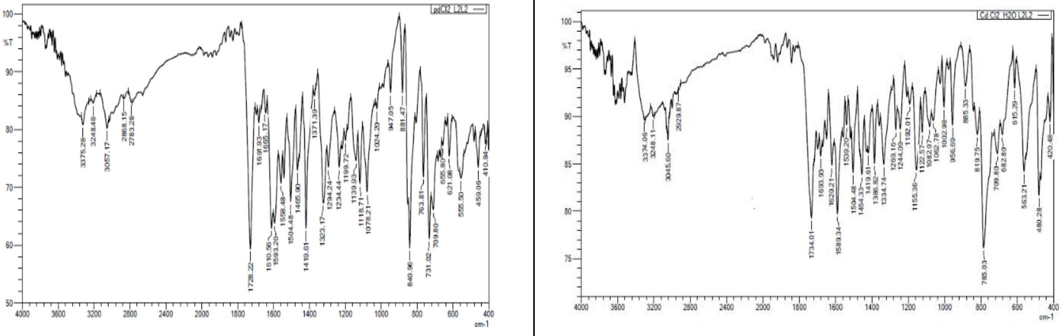
Compound	**v C=O**	**v C=O istain**	**v C=N**	**v C=N 1,10-phen**	**v NH v NH$_{(istain)}$**	**v M-O**	**v M-N**	**vM-Cl**
L	1732	1676	1624	----	3244 3375	-----	------	-------
1,10-phen				1597				-------
[Cr(L)1,10-phen Cl_2]Cl	1732	1686	1640	1618	3252 3379	563	460	383
[Mn(L)1,10-phen Cl_2]	1732	1686	1638	1606	3245 3373	563	547	318
[Zn(L)1,10-phen]Cl_2	1732	1691	1649	1622	3245 3375	563	516	------
[Pd(L)1,10-phen]Cl_2	1728	1691	1665	1610	3248 3375	555	459	-------
[Cd(L)1,10-phen]Cl_2	1734	1693	1660	1620	3248 3374	563	480	------
[Pt(L)1,10-phen Cl_2]Cl_2	1730	1697	1649	1620	3242 3371	553	457	318



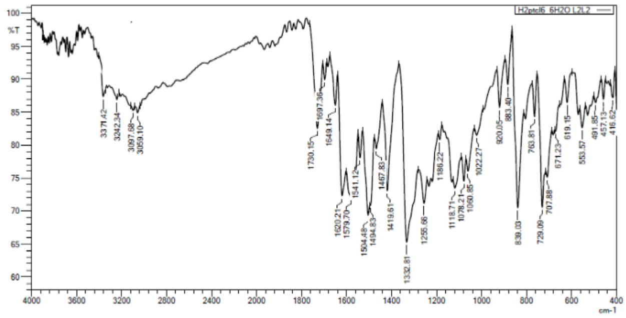
(a) L (b) Cr complex



(c) Mn complex (d) Zn complex



(f) Pd Complex (g) Cd complex



(h) Pt complex

Figure 3: FTIR spectra for L and complexes

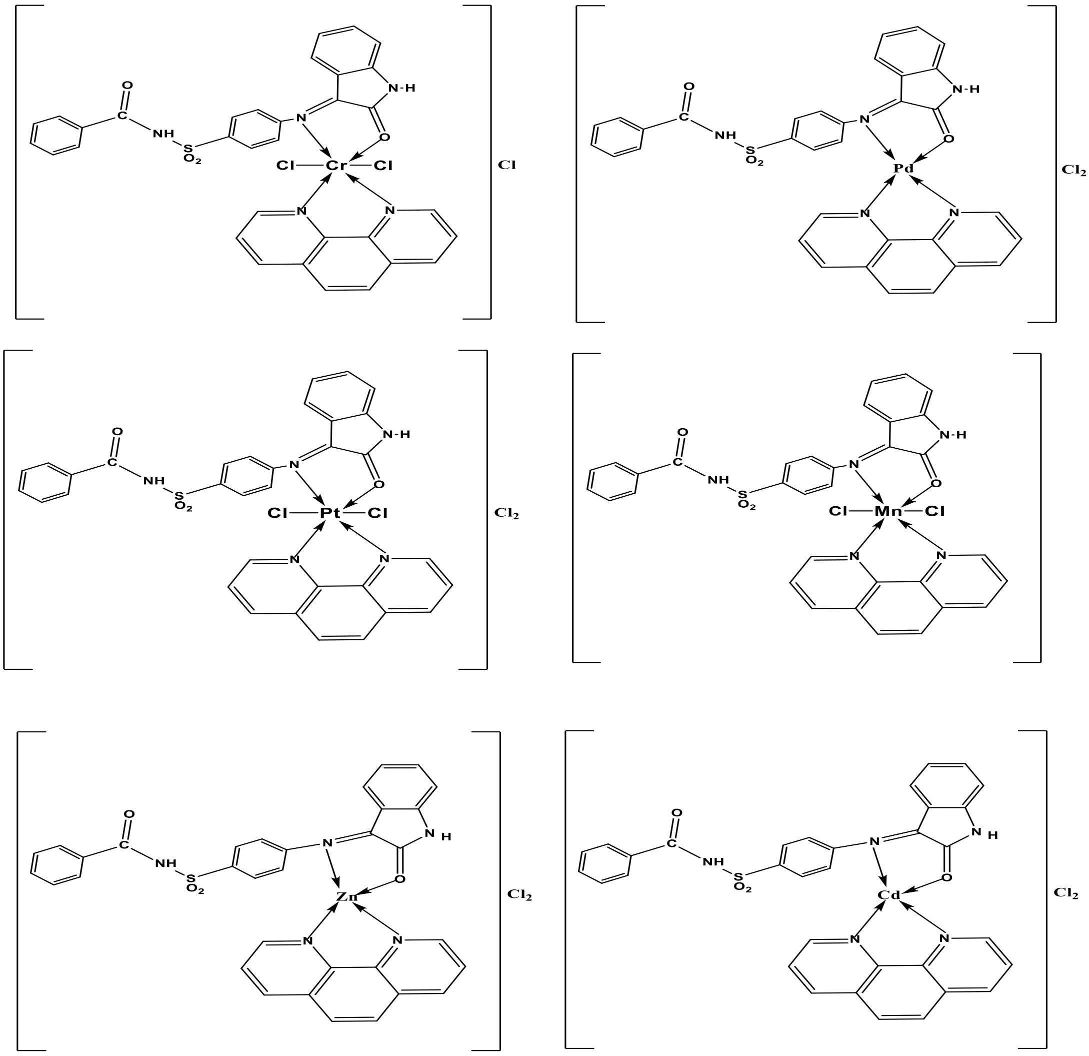


Figure 4: Suggested forms of prepared complexes

3.5. ^{1}H-NMR and ^{13}C-NMR for ligand and 1,10-phen

^{1}H-NMR spectrum

The ^{1}H-NMR spectrum of new (L) , recorded in DMSO - d_6, shows a signal at (2.47) ppm attributed to (H_2O). Multiple signals appeared at the range (6.16-7.93)ppm, corresponding to the proton of the aromatic ring of phenyl ring (m, H-Ar, phenyl ring), and two signals belonged to singlet proton of two groups NH presented in the ligand (S, H, of NH) at (11.03,12.10) ppm [28,29]

In 1,10-phenanthroline the protons of aromaticity of C=N appeared at 9.14 ppm. Other bands can be seen in Table 4.

^{13}CNMR Spectrum

The NMR spectrum of carbon 13 of the (L) and 1,10-phenanthroline was recorded in the solvent of dimethyl sulfoxide –d_6, with chemical shifts in ppm. The ligand showed several signals attributed to the carbon aromatic ring of benzene groups at 112.64-138.82, while a signal appeared at 159.84 ppm, which is attributed to carbon in (C=N) of the imine group [30]. The signals that appeared at 151.16, 154.16 ppm belong to the carbon of C-N group, a signal appeared at 165.53 ppm belonging to the carbonyl of istain group, and another single band at 184.86 ppm attributed to the carbon of carbonyl sulfabenzamide. In 1,10-

phenanthroline the carbon of C=N appeared at 151.41 ppm [31]. Other bands can be found in Table 4.

Table 4: (^{1}H) & (^{13}C) NMR spectra of two ligands (L) and 1,10-phenanthroline

^{1}**H-NMR**	^{13}**C-NMR**
L ^{1}H-NMR(DMSO- d6) δ ppm: 2.47 (H_2O), 6.16-7.93 (m,H-Ar,phenyl ring),11.03,12.10(S,H, of NH groups).	L ^{13}C-NMR(DMSO-d6) δppm:112.64-138.82 (carbon of aromtic ring of benzene groups), ring),151.16,154.16(carbon of C-N group) ,159.84 (carbon of C==N of imine group),165.53 (carboyl of istain)184.86 (carbon of carbonyl sulfabenzamide).
1,10-phenanthroline ^{1}H-NMR(DMSO-d6) δ ppm: 7.67-8.53(m, H-Ar, phenyl ring) of 1,10-phenanthroline , 9.12,9.14(S,HC=N) , 2.5 of DMSO solvent .	**1,10-phenanthroline ^{13}C-NMR(DMSO-d6) δ ppm :** 124.26, 126.66 ,133.26,136.21,140.42 (Carbon of aromatic ring), 151.41 (carbon of HC= N group) .

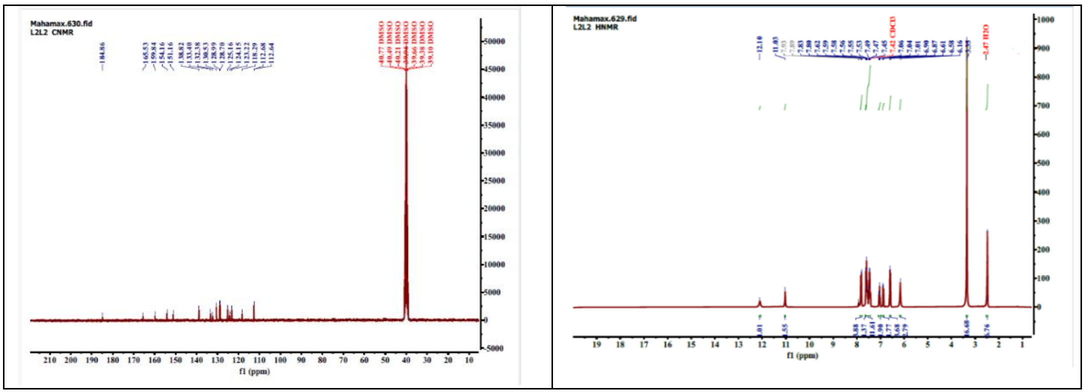
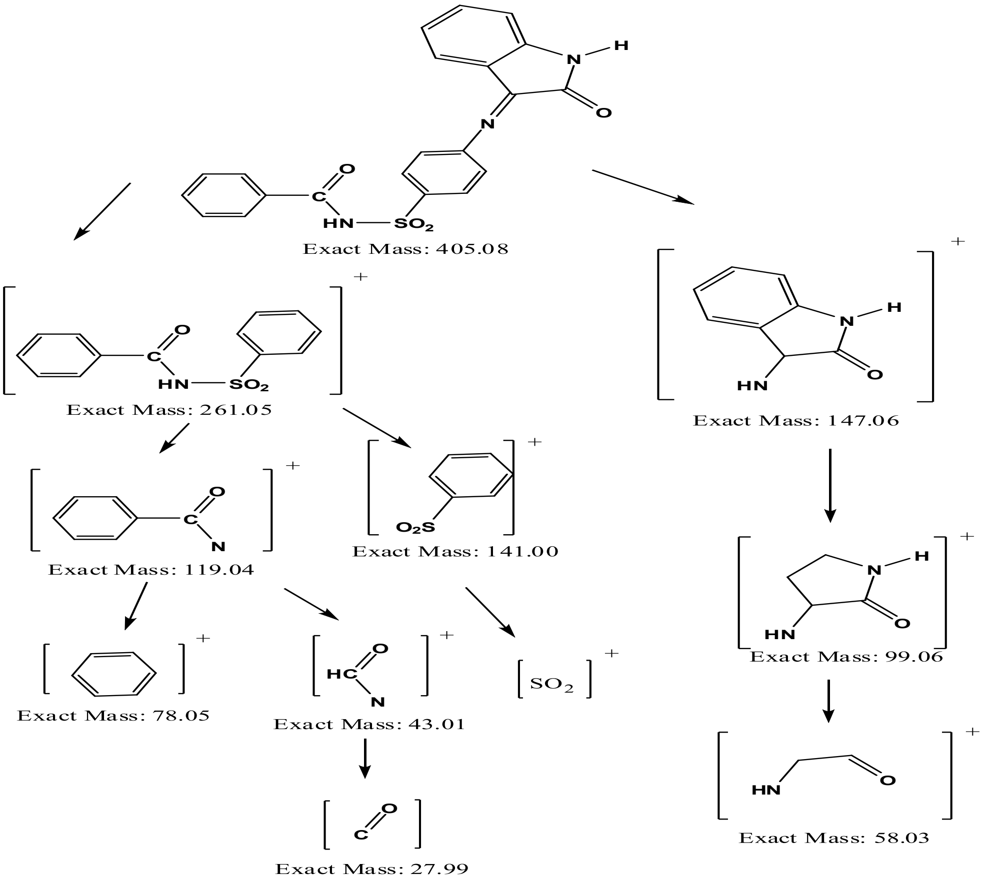


Figure 5: :^{1}HNMR and ^{13}CNMR spectra for L

3.6. Mass spectra of ligand(L)

The mass spectrum of the Schiff base ligand (L) N-(4-(2-oxoindoline-3-ylideneamino) phenylsulfonyl) benzamide, displays a prominent peak at m\z=405.0, corresponding to the molecular weight of the empirical formula.C21H15N3O4S The peak of the fragments at 261 m/z is attributed to the formula [C13H11O3NS)+,20].

Additional fragments peak at147m/z[C8H6N2O,+25],119m/z[C7H5NO,+70],141m/z[C6H5O2S,+55],99m/z[C4H4N2O,+40],43m/z[CHNO,+20],78 m/z[C6H6,+100],58 m/z[C2HNO,+50],27m/z[CO,+18] [32, 33].



Scheme 2: The spectrum mass of fragments for L

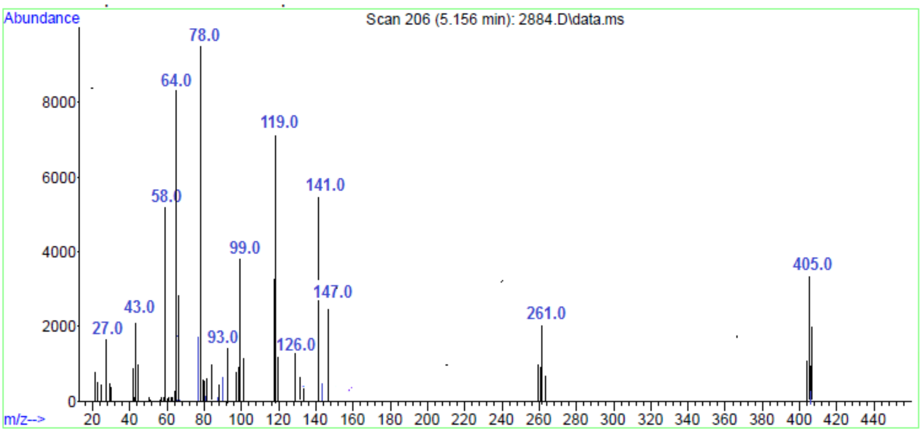


Figure 6: Mass spectrum for L

3.7. Biological Activity of mixed ligands complexes.

The diameter of the inhibition zone for ligands and all mixed ligands complexes by disc diffusion method was measured using the solvent DMSO at a concentration of 0.02 M and amoxicillin as the standard drug for bacteria and fluconazole for fungi, Table 5. Overall, all biologically tested compounds showed significant activity against selected types of negative and positive bacteria as well as fungi when compared to standard drugs. The Schiff bases complexes with chromium, zinc and palladium complexes showed high inhibitory activity against *Spatphylococcus* bacteria compared to the prepared ligand and the standard drug, while the chromium complex showed the highest bacterial activity against *Bacillus*, and the palladium and platinum complex showed the highest bacterial activity against *E. coli* negative bacteria compared with the rest complexes and the standard drug, the manganese and palladium complexes showed the highest bacterial activity against negative *Acinetobacter baumannii* bacteria compared to the rest of the complexes and the standard drug, while most of the complexes had high inhibitory activity against *Candida* fungi compared to the standard drug. In contrast, the standard medication did not demonstrate any effectiveness against all tested bacteria and fungi. [34,35].

Table 5: Inhibition zone (mm) of (L), 1,10-phen and metal complexes at 0.02M.

Types of bacteria and fungi						
Compounds		**Types of positive bacteria**		**Types of negative bacteria**		**fungi**
		Staphylococcus	***Bacillus***	***E.coli***	***Acinetobacter baumannii***	***Candida***
1	L	25	-	29	22	35
2	1,10-phen	11	17	18	11	18
3	[Cr(L)1,10-phen Cl_2]Cl	50	47	25	26	25
4	[Mn(L)1,10-phen Cl_2]	30	40	30	50	40
5	[Zn(L)1,10-phen]Cl_2	54	40	28	31	40
6	[Pd(L)1,10-phen]Cl_2	55	44	45	50	40
7	[Cd(L)1,10-phen]Cl_2	18	15	27	31	28
8	[Pt(L)1,10-phen Cl_2]Cl_2	40	43	44	40	39
9	Amoxicillin For bacteria	-	-	15	-	-
10	Flucananzole For fungi control	-	-	-	-	-

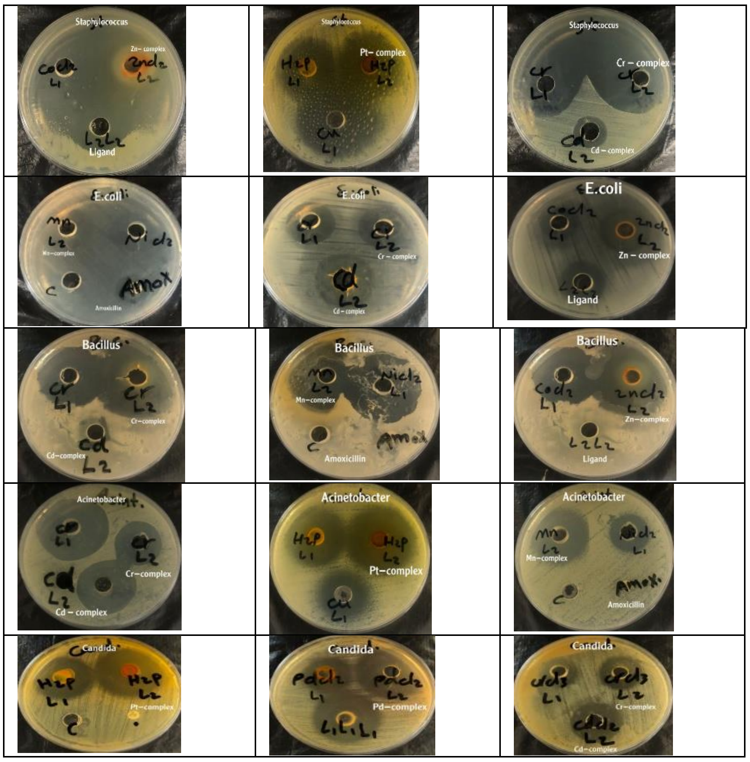


Figure 7: Types of bacteria and fungi

3.8. Theoretical study

The Hyperchem-8.0.7 program was used to analyse the ligands and their complexes in their theoretical study. Table 6 presents the standard heat of formation and bonding energy for each synthesized chemical determined by the PM3 method for Cr, Mn, Zn, and Cd complexes and the AMBER method for Pd, and Pt complexes. The data indicated that the complexes exhibited a high degree of stability, as shown in Table 6. Vibration frequencies were calculated using hyper program. A comparison between theoretical and experimental results was made, revealing the percentage of error between them as shown in Table 7 and Figure 9. Also calculated the active groups in the molecule were studied by identifying the HOMO, LUMO. The electrostatic potential can be calculated, as shown in Figure 10 [36].

Table 6: Thermodynamic factor (in KJ.mol^{-1}) utilizing the HyperChem-8.0.7in different methods of all prepared compounds

PM3			**AMBER**
Comp.	**ΔH°_f**	**ΔE_b**	**$\Delta H^\circ_f = \Delta E_b$**
L	-5327.4592233	-38.5092233	
[Cr(L)1,10-phen Cl$_2$]Cl	-169.9977582	-8305.4237582	
[Mn(L)1,10-phen Cl$_2$]	-127.2943903	-8235.4203903	
[Zn(L)1,10-phen]Cl$_2$	-85.8200139	-7927.7959861	
[Pd(L)1,10-phen]Cl$_2$	------	-------	73.316403
[Cd(L)1,10-phen]Cl$_2$	-115.9429530	-7893.2230470	
[Pt(L)1,10-phen Cl$_2$]Cl$_2$	-----------	---------	232.436673

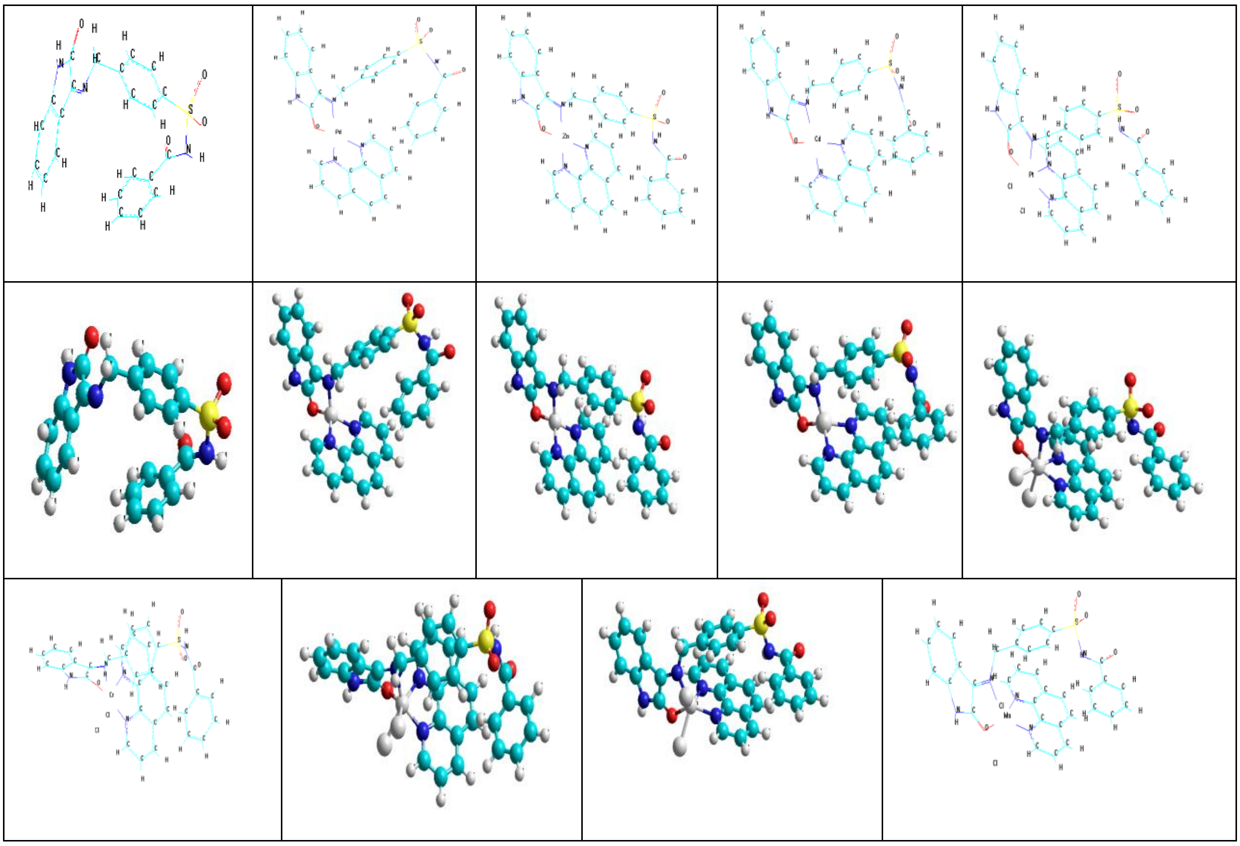


Figure 8: Stable geometry of all mixed ligands complexes

Table 7: Comparison between practical and theoretical results using hyperchem program and determining the error rate between them

Symb.	ν(C=N)1,10phen.	ν (C=N)	**νC=O** istain	**νC=O**	**νNH**
Experimental	1597	1624	1676	1732	3244 3375
Theoretical	*1624	*1647	*1684	*1770	*3265 *3421
Percentage of error	(1.66)	(1.39)	(0.47)	(2.14)	(0.64) (1.34)

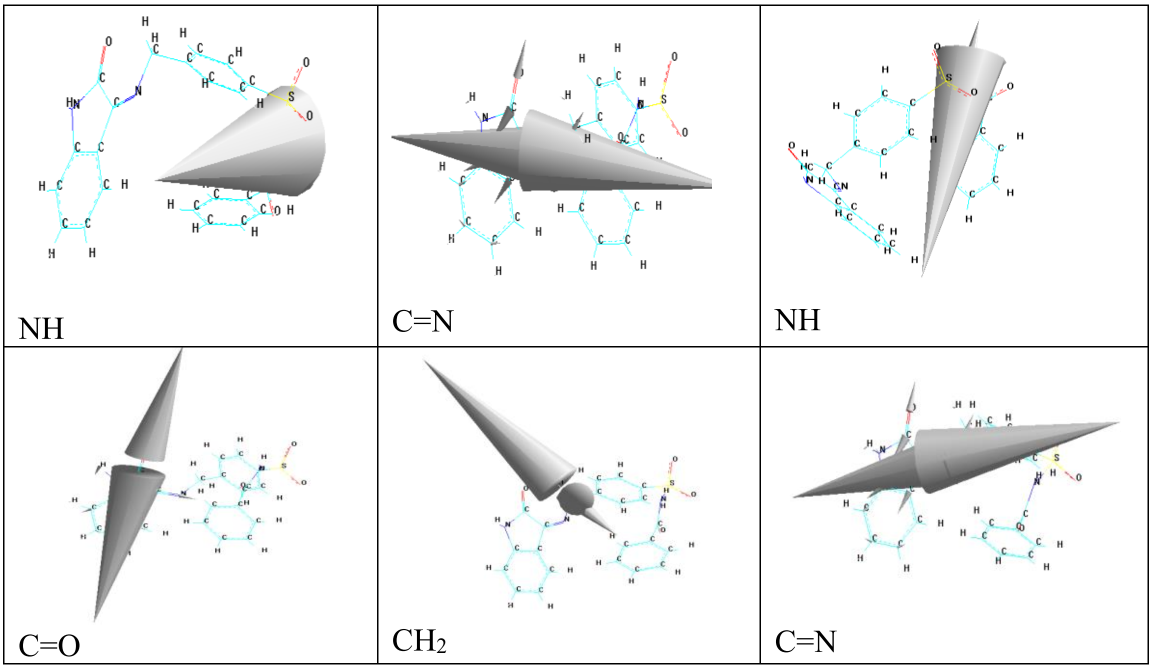


Figure 9: The vibration frequencies of active group in ligand(L)

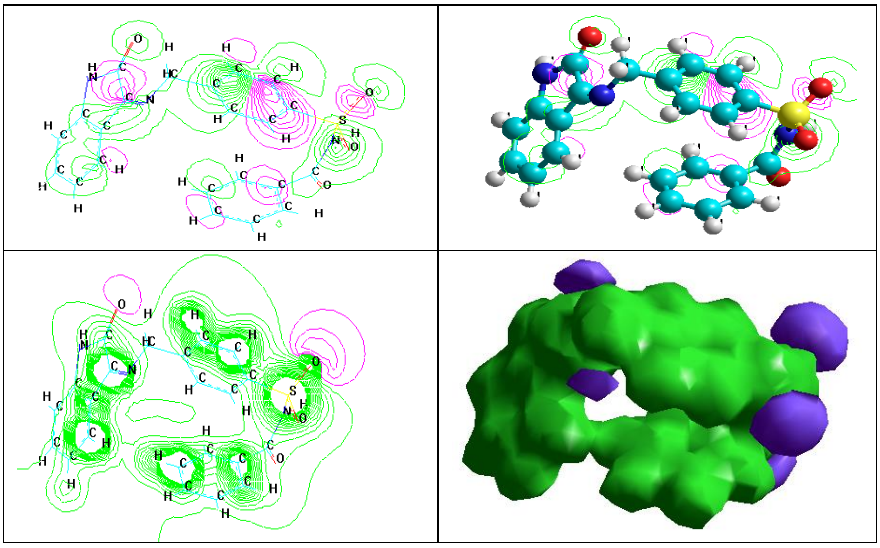


Figure 10: Electrostatic potential, HOMO &LUMO in different dimensions for ligand

Conclusions

In this study, a new Schiff base derived from sulfabenzimide was synthesized. A series of mixed ligand complexes with metal ions of varying valences were prepared using the Schiff base and 1,10-phenanthroline. All synthesized compounds were characterized by the following spectroscopic methods, elemental analysis, FT-IR, and UV-Vis except for proton and carbon resonance spectra, mass spectra (^{1}H-NMR,^{13}C-NMR and GC-MS), which were for ligands only, conductivity, and magnetic susceptibility of the complexes. The results showed that mixed ligands complexes of chromium, manganese, and platinum have an octahedral geometry, while zinc and cadmium complexes have a tetrahedral geometry. The palladium complex is characterized by a square planar geometry, with coordination from the Schiff base ligand (L) and 1,10-phenanthroline acting as bidentate ligands. The complexes prepared in solution were studied to determine the ratio of the metal to the ligand using the molar ratio method. The study proved that the complexes are coordinated with the ligands in a ratio of 1:1.1. IR measurements revealed that the ligands exhibit a bidentate with all metal ions. Complexation takes place in N and O atoms. The biological activity of all compounds was studied using two types of positive bacteria, two types of negative bacteria, and one type of fungi, using the standard drugs as a reference. The results demonstrated that the complexes exhibited significant inhibitory activity compared to the standard drugs.

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