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Biological Evaluation and Theoretical Study of Bi-dentate Ligand for Amoxicillin Derivative with Some Metal Ions

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Abstract:

In this paper, the complexes of Shiff base of Methyl -6-[2-(diphenylmethylene)amino)-2-(4-hydroxyphenyl)acetamido]-2,2-dimethyl-5-oxo-1-thia-4-azabicyclo[3.2.0]heptane-3-carboxylate (L) with Cobalt(II), Nickel(II), Cupper(II) and Zinc(II) have been prepared. The compounds have been characterized by different means such as FT-IR, UV-Vis, magnetic moment, elemental microanalyses (C.H.N), atomic absorption, and molar conductance. It is obvious when looking at the spectral study that the overall complexes obtained as monomeric structure as well as the metals center moieties are two-coordinated with octahedral geometry excepting Co complexes that existed as a tetrahedral geometry. Hyper Chem-8.0.7 program was employed, after calculating the heat of formation **(ΔH_f)**, binding energy **(ΔE_b)**, dipole moment(μ), and FT-IR frequencies are carried out in gas phase, the geometric shape is suggested. The compounds have been also screened for their bioactivity to antibacterial and antifungal.

Keywords: Biological activity, Complexes of Schiff base, Schiff base ,Theoretical study

Introduction:

The significance of nitrogen-containing complexes in their application as high-efficiency biopharmaceuticals to many fungi is significant, for nitrogen possesses a high degree of consistency with metal in a base or neutral medium because it owns a single electronic pair that can be shared with another atom (1) .Schiff bases form a crucial class of the best and extensively used organic compounds and have a wide range of applications in numerous fields comprising analytical and biological fields (2). Schiff bases have distinction in medicinal and pharmaceutical arenas due to their expansive spectrum of biological activity such as antibacterial, antifungal (2, 3), anticancer (4) and herbicidal activities (5). Amoxicillin ($C_{16}H_{19}N_3O_5S$) is a semi synthetic penicillin type antibiotic which has little effect toward gram-negative bacteria and high effect toward gram-positive bacteria (6). It is used in human medicine as well as in veterinary practice. The presence and fate of amoxicillin in the environment have been investigated. Studies available in the scientific literature stated that, although usually detected in trace concentrations, amoxicillin continuous release into the environment surges the possibility of synergistic effects with other pharmaceuticals or chemicals in the aquatic effluent (7, 8). Studying coordination chemistry concerning transition metal ions with some types of ligands has been improved by the present advancements in medicine and bioinorganic chemistry (9). This work describes the process of synthesizing a new Shiff -imine ligand along with its Cu(II), Co (II) , and Ni (II), Zn (II) coordination compounds. The new synthesized compounds have been characterized by means of some spectral procedures. Biological activities of compounds have been tested by using two bacterial types.

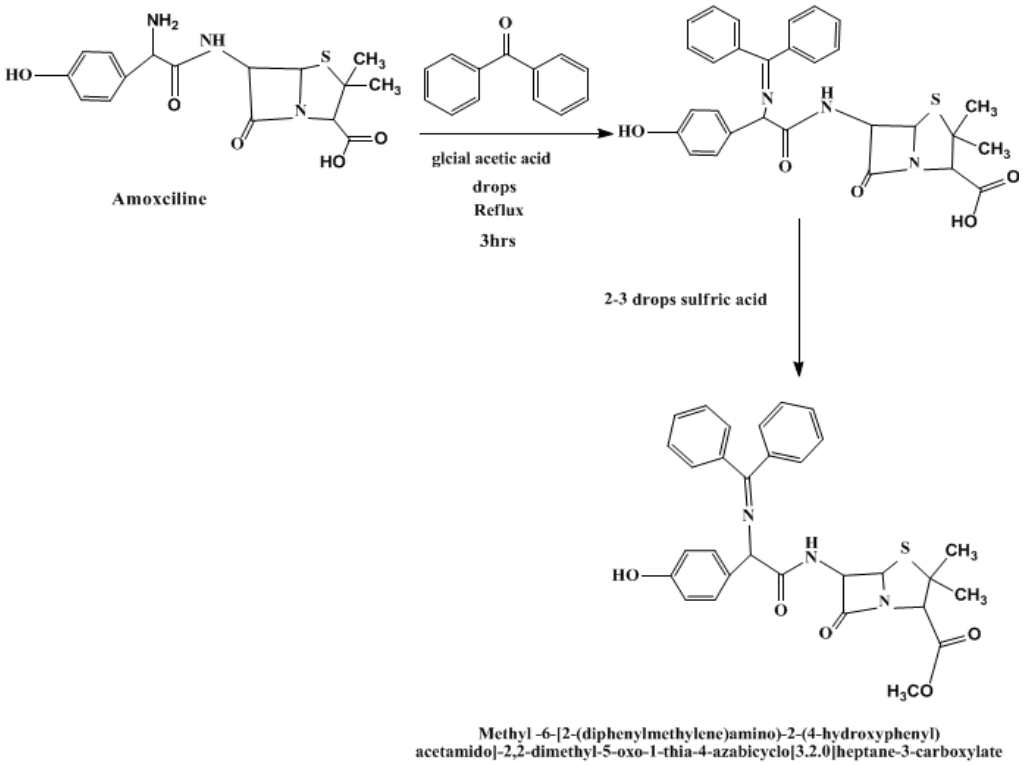
Materials and Methods:

All metal salts used in this work have been obtained from Fluka ($CoCl_2.6H_2O$, $NiCl_2.6H_2O$,

$CuCl_2.2H_2O$ and $ZnCl_2$). FTIR spectra have been recorded on Shimadzu8400 and wave number is ranged for 4000-200 cm^{-1} ,Uv-Vis 1600A Shimadzu has been used as a means of recording the electronic spectra at wave length ranged of 190-1100 nm. The metal analysis has been conducted via a Perkin Elmer 500 Atomic Absorption Spectrophotometer. Conductivity Meter 220 with Gallen camp has been used to calculate the molar conductivity in DMF as a solvent at room temperature in concentration 10^{-3} M, M.F.B-600.01 as a melting device. Magnetic susceptibility balance model MSB-MKT has been used for magnetic moment measurement.

The Rout of the Preparation for the Ligand

In round bottom flask, (150 ml) a mixture of (0.01) mole amoxicillin and benzophenone with an excess of absolute methanol with (4-5) drops of anhydrous acetic acid was placed. After that the solution was refluxed for six hours. The resulting precipitate obtained was dried, and re-crystallized using ethyl alcohol solvent, and then some drops of concentrated sulfuric acid were added. The mixture was refluxed for three hours. The precipitate obtained was filtered, dried, and next re-crystallized from ethyl alcohol (10).The steps for preparing the ligand are shown in **Scheme 1**



Scheme 1. Steps of the synthesis of ligand (L)

Preparation of Complexes:-

To prepare the complexes (0.236, 0.237, 0.170 and 0.32 g) of $CoCl_2.6H_2O$, $NiCl_2.6H_2O$, $CuCl_2.2H_2O$ and $ZnCl_2$ were dissolved in 10 ml of ethanol for each, and then mixed with (0.93) g of ligand that was dissolved previously in 15 ml ethanol in a molar ratio 1:1, then they were refluxed for 3 hours. The precipitates, which were colored and then were filtered, were washed using hot ethanol and finally dried using desiccators at $60^{O}C$.

Results and Discussion:

Divalent metal salts have been estimated using atomic absorption technology in order to determine the ratios of these elements. Some measurements such as the melting point and the percentage of the yield are implemented for the sake of proposing the structural formulas of the prepared complexes as illustrated in **Table 1**. The molar conductivity of the complexes has been measured as well via using DMF as solvent at room temperature.

The physio-chemical properties are summed up in **Table 1**. The complexes are characterized with stability at room temperature with various melting points and different colors.

Table 1. Analytical and some physical data for the ligand and its metal complexes

Compounds	Elemental analysis Found , (Cal.) %				M.P ^{O}C	Color	% Yield	μ_{scm}^{-1}
	C	H	N	M				
L	67.33 (65.77)	5.33 (5.14)	8.28 (7.39)	---	196	Bulbous	77%	----
Co-L	52.68 (53.57)	3.99 (4.31)	6.50 (6.25)	9.12 (8.76)	177	Greenish Blue	76%	18.20
Ni-L	50.03 (50.84)	3.83 (4.66)	6.11 (5.93)	9.29 (8.28)	205	pale yellow	73%	16.44
Cu-L	48.33 (49.24)	3.93 (4.78)	5.00 (5.74)	7.68 (8.68)	213	Green	66%	12.67
Zn-L	50.62 (50.34)	3.75 (4.61)	4.99 (5.87)	8.79 (9.14)	225	Yellow	78%	14.98

The ligand has been identified by using infrared spectroscopy, where the spectrum has revealed a band at 3268 cm $^{-1}$ which is attributed to the NH group and a band at 1779,1732 ,1176, 1388 cm^{-1}, dating to the υ C = O group of ester, β-lactam, υ CSC and υ C-N sequentially (11). The spectrum also has displayed a wide beam at 3450 cm^{-1}, which is attributed to the presence of water in the ligand. Also, there were bundles present at 1600 and 1582 cm^{-1} which attributed to υ (C=N) and υ (C=C) that remains constant and no change in the complexes .

In complexes, the displacement of the values of the υ C-N is towards the lower frequencies than in the ligand but, the bands of υ CSC and υ C=O of β-lactam remained constant in the complexes (12), this shift confirms the coordination of the nitrogen atom of β-lactam group to the metal ions. The band at 1779 cm^{-1} of υ (C=O) ester group is shifted in all complexes, therefore oxygen of carbonyl υ C=O takes place in coordination. This supports the compatibility with the C=O group (13).The bands have been observed at(3400-3450) cm^{-1} which attributed to the stretching frequencies of OH change in Ni^{+2},Cu^{+2} and Zn^{+2} complexes, give evidence of the presence of (H_2O) molecules in coordination sphere. They also display the existence of some weak bands available in 905–918 range which is due to coordinated water (14). A non-ligand band can be seen in the region (530–578) and (472-478) cm^{-1} in all the complexes that have been assigned to υ (M-N) and υ (M-O) sequentially (14). Thus, for displaying the above discussion, the general structures for the metal complexes are illustrated in **Table 2**.

Table 2. Fourier transform infrared spectroscopy bands of compounds

Comp.	$\nu_{C=N}$	$\nu_{C=C}$	ν_{NH}	ν_{C-N}	$\nu_{C=O}$ β-lactam est.	ν_{C-S-C}	ν_{C-S}	$\nu_{C-H\ Alp.}$	$\nu_{CH\ Orom.}$	ν_{M-N}	ν_{M-O}
L	1600	1582 1512	3268	1388	1732 1779	1176	765	2962 2927	3055	----	----
CoL	1600	1599 1510	3262	1372	1731 1759	1178	756	2970 2933	3047	530	477
NiL	1600	1582 1515	3265	1375	1732 1754	1178	763	2984 2962	3000	543	478
CuL	1608	1598 1516	3262	1376	1730 1750	1178	759	2999 2960	3035	578	472
ZnL	1602	1586 1516	3266	1376	1731 1753	1178	755	2986 2963	3024	544	472

The Uv-vis spectrum of the ligand demonstrates two bands at (38314) and (20964) cm^{-1} which attributed to ($\boldsymbol{\pi - \pi^*}$) transition of (C=C) group and ($\boldsymbol{n - \pi^*}$) may be situated on the (C=O) group (14).

Electronic spectra of complexes in Table 3, reveal electronic transition bands to the ligand and its complexes. The regular transition bands of Co (II) complexes are three bands ν_1: $^4A_{2\ (F)} \rightarrow {}^4T_2$ ν_2: $^4A_2 \rightarrow {}^4T_{1\ (f)}$, $\nu 3$:$^4A_2 \rightarrow {}^4T_{1\ (p)}$ at 4329, 7561, 15128 respectively which attributed to tetrahedral geometry (15, 16), **Fig. 1.**

Electronic spectrum of Ni (II) complex displays bands in 9837, 18092 and 23426 ranges which have been assigned to the transitions, $^3A_2g \rightarrow {}^3T_2g_{(f)}$, $^3A_2g_{(f)} \rightarrow {}^3T_1g_{(f)}$ and $^3A_2g_{(f)} \rightarrow {}^3T_1g_{(p)}$,which indicates that the complex is octahedral(15,16), **Fig. 1.**

Uv-vis spectrum of Cu(II) complex displays bands in the position 48540 and 43471 cm^{-1} which have been attributed to the charge transfer. Also, other bands appeared at 15974 cm^{-1} as abroad band correspond to $^2Eg \rightarrow {}^2T_2g$ transition, the emergence of the broad cupper band is due to the influence of John-Tellar (15, 17), **Fig 1**.

Finally, the electronic spectrum of yellow Zn (II) complexes has one band at 42325cm^{-1} which can correspond to the C-T and also two bands at 34278 and 21346 cm^{-1} which attributed to the $(\pi - \pi^*)$ and $(n - \pi^*)$ transitions(15,9) ,the geometry of this complex can be observed in **Fig. 1**.

Table 3. Uv-visible bands of prepared compounds

Comp.	Absorption Bands cm^{-1}	Transitions	*μeff B.M.*
L	20964	n-π^*	
	38314	π-π^*	----
Co-L	4329	$^4A_{2\ (F)} \rightarrow {}^4T_2$	
	7561	$^4A_2 \rightarrow {}^4T_{1\ (f)}$	4.81
	$15128_{(av.)}$	$^4A_2 \rightarrow {}^4T_{1\ (p)}$	(3.87)
Ni-L	9837	$^3A_2g \rightarrow {}^3T_2g_{(f)}$	
	18092	$^3A_2g_{(f)} \rightarrow {}^3T_1g_{(f)}$	3.39
	23426	$^3A_2g_{(f)} \rightarrow {}^3T_1g_{(p)}$	(2.82)
Cu-L	15974	$^2Eg \longrightarrow {}^2T_2g$	
	43471	Charge Transfer	1.80
	48540	Charge Transfer	(1.73)
Zn-L	21346	n-π^*	
	34278	π-π^*	0.00
	42325	Charge Transfer	

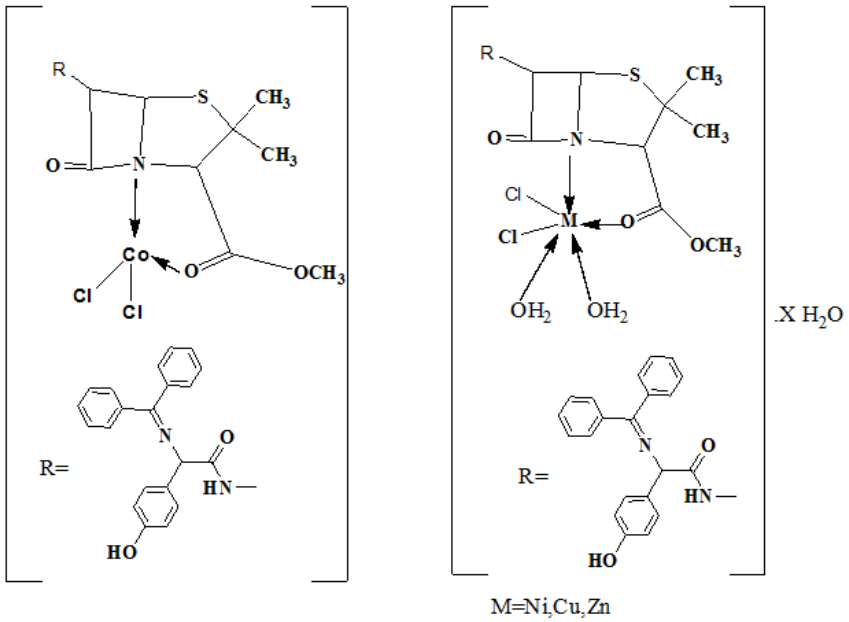


Figure 1. Geometries of complexes

Antibacterial and Antifungal Activities:

Pathogenic microorganisms cause diverse kinds of ailments to both human as well as animals. The detection of chemotherapeutic agents has a very vital part in controlling and preventing such ailments. The microorganisms are able to grow resistance toward those chemotherapeutic agents and these strains which are resistant triggering an essential problem in the treatment of microbial infections. Searching for new antimicrobial agents gets to be very indispensable; therefore excessive efforts have been engaged to discover different antibiotics or novel compounds with worthy antimicrobial activity which could be proper to be utilized as chemotherapeutic agents (18, 19).

In this study, all prepared compounds have been evaluated *in vitro* as antimicrobial of two types (gram negative and gram positive) bacteria, Gram positive (*Staphylococcus aureus)* and Gram negative bacteria (*Echerchia coli)* and *antifungal* (*Candida albicans*) effect. However, all prepared compounds have a good inhibiting effect

on bacteria and fungi, with the exception of zinc complexes which show no effect of inhibition on the bacteria and fungi assessed, it may be because electronic configuration or geometry shape, **Table 4**.

Table 4. In vitro inhibition compounds toward gram- positive and gram- negative in two concentrations

Comp.	*Staphylococcus aureus*		*Escherichia Coli*		*Candida albicans*	
	5mM	*10mM*	*5mM*	*10mM*	*5mM*	*10mM*
L	+	++	++	+	+	+
Co L	+++	+++	+	++	+	++
Ni L	-	+	++	++	+	++
Cu L	+	++	+	++	+	+
Zn L	-	+	-	-	-	+
EtOH	-	-	-	-	-	-

(-): Show no inhibition effect
(+): Show little inhibition effect
(++): Show moderate inhibition effect
(+++): Show good inhibition effect

Studying of Complexes Formation in Solution:

New complexes of Schiff base of divalent ion Co, Ni, Cu and Zn have been studied in solution using ethyl alcohol as a solvent, to determine the ratio of metal to ligand at λ_{max}. The results have shown that the metal ions are coordinated with the ligand by ratio (1:1) according to the **Fig. 2** .

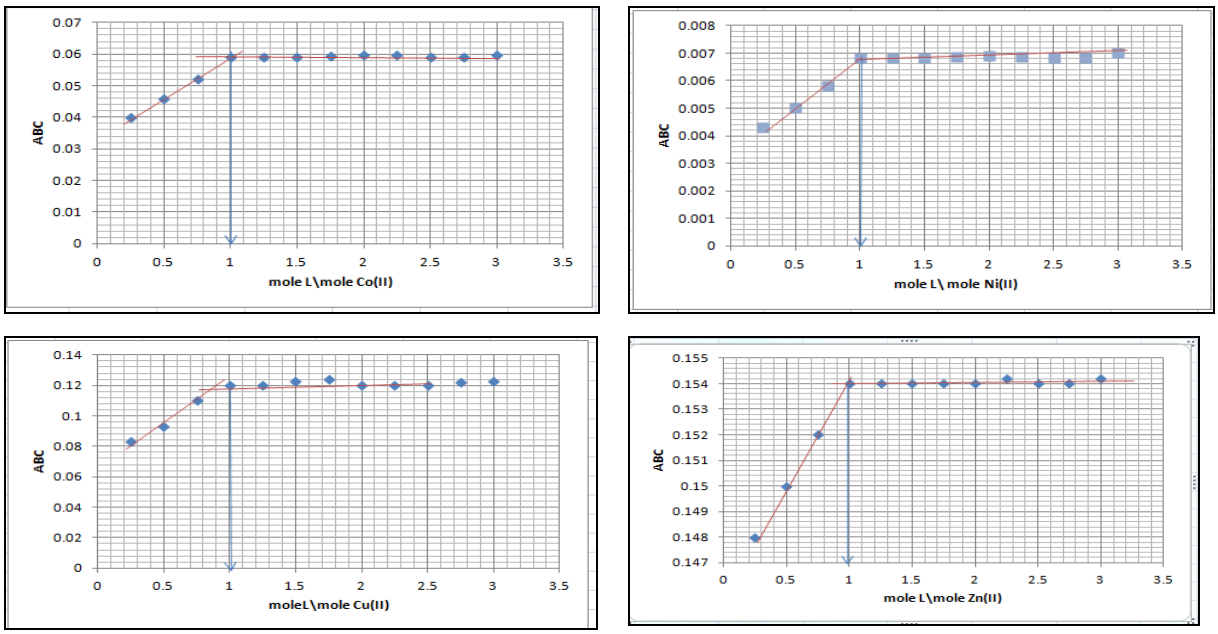


Figure 2: The molar ratio plot of metal complexes

Theoretical Calculations

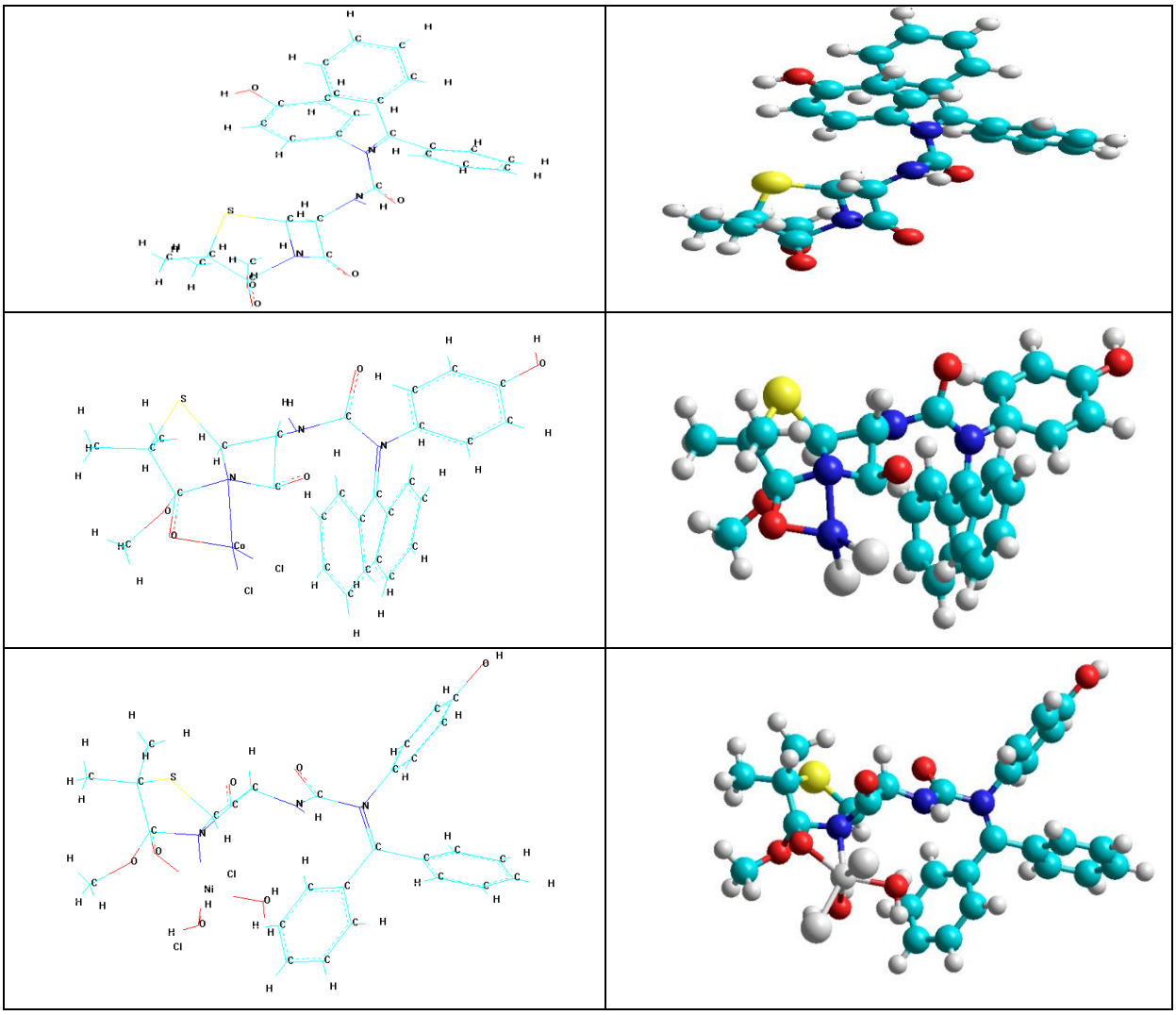
The program utilized in theoretical treatment is Hyper chem-8.0.7.The heat of formation and banding energy have been calculated by using two methods: the first is PM3 and the second is ZINDO\1 for both the ligand and the prepared complexes in order to show their stability. Next, the most stable geometry of all the prepared compounds is obtained, **Table 5**, **Fig. 3** in addition to the calculation of the vibrational frequencies of ligand theoretically and comparing the experimental results with the calculation of the error rate between the two used methods, **Table 6 and Fig. 4**, also **Figs. 5** and **6** show HOMO, LUMO of ligand (L) and bond length of prepared compounds.

Table 5. Heat of formation ($\Delta H_{\circ f}$),binding energy (ΔE_b) and dipole moment(μ) for Ligand and it's metal complexes using the program hyperchem-8.0.7

Comp.	PM3			ZINDO/1		
	$\Delta H°_f$	ΔE_b	μ	$\Delta H°_f$	ΔE_b	μ
L_1	16.9321466	-6877.9368534	22.97	-14339.4214187	-21234.2904187	3.41
CuL	-267.0956459	-7628.1706459	11.5	-15167.4214722	-22528.4964722	7.23
NiL	-393.0699911	-7776.2449911	6.47	-14664.3881614	-22047.5631614	7.18
CoL	-369.3128454	-7424.5618454	17.77	-14170.4340856	-21225.6830856	18.03
ZnL	-210.3641765	-7521.9091765	27.71	-15227.2865644	-22538.8315644	25.22

Table 6. The frequencies of ligand using the program hyper chem.-8.0.7

Type of method	N (C=N)	V (C-N)	v (C=O) of ester	ν(C-H)aliph.	ν(C-H) *aromatic*	v CS	V CSC	V *NH*
Experimental	1600	1388	1779	2962 2927	3055	765	1176	3220
Theoretical	1656	1331	1799	3005 2900	3022	711	1197	3312
Error%	(3.38)	(-4.28)	(1.11)	(1.43) (-0. 93)	(-1.09)	(-7.59)	(1.75)	(2.77)



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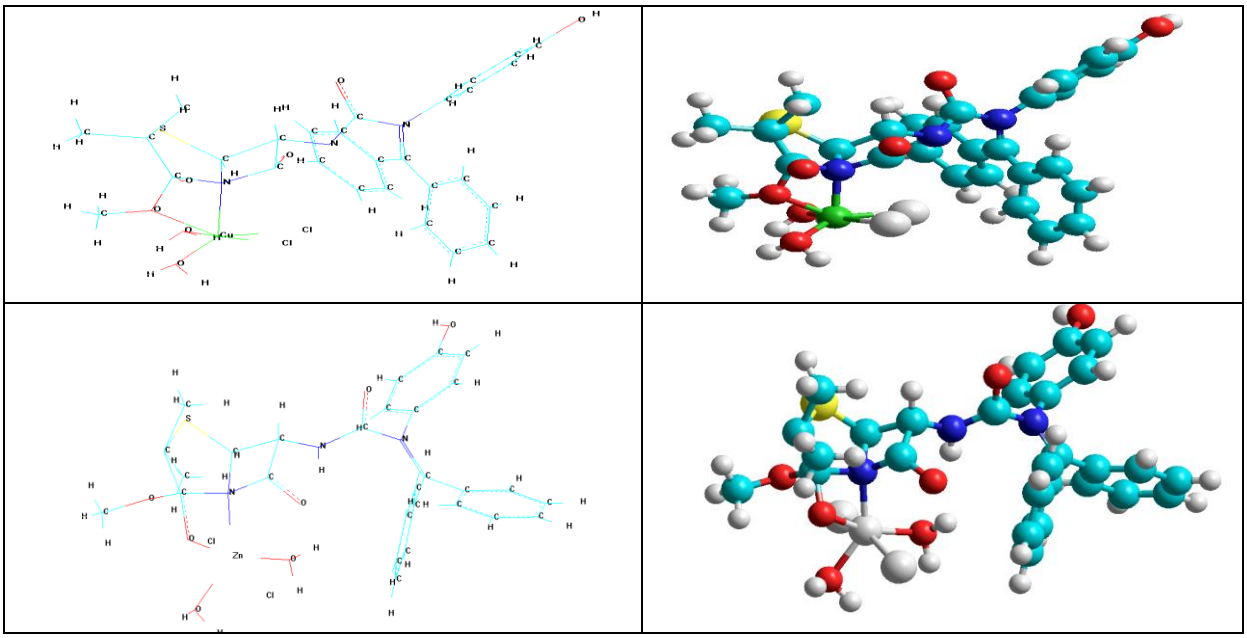
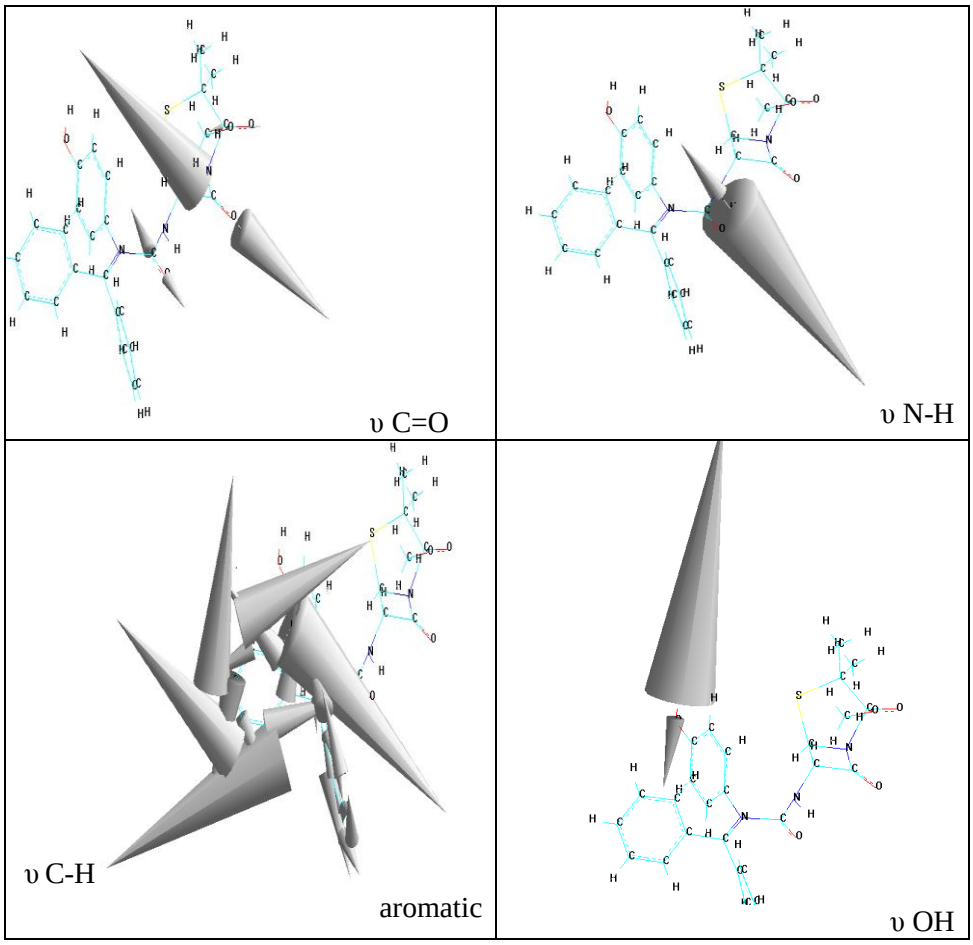


Figure 3. Geometries of ligand and divalent metal ion complexes



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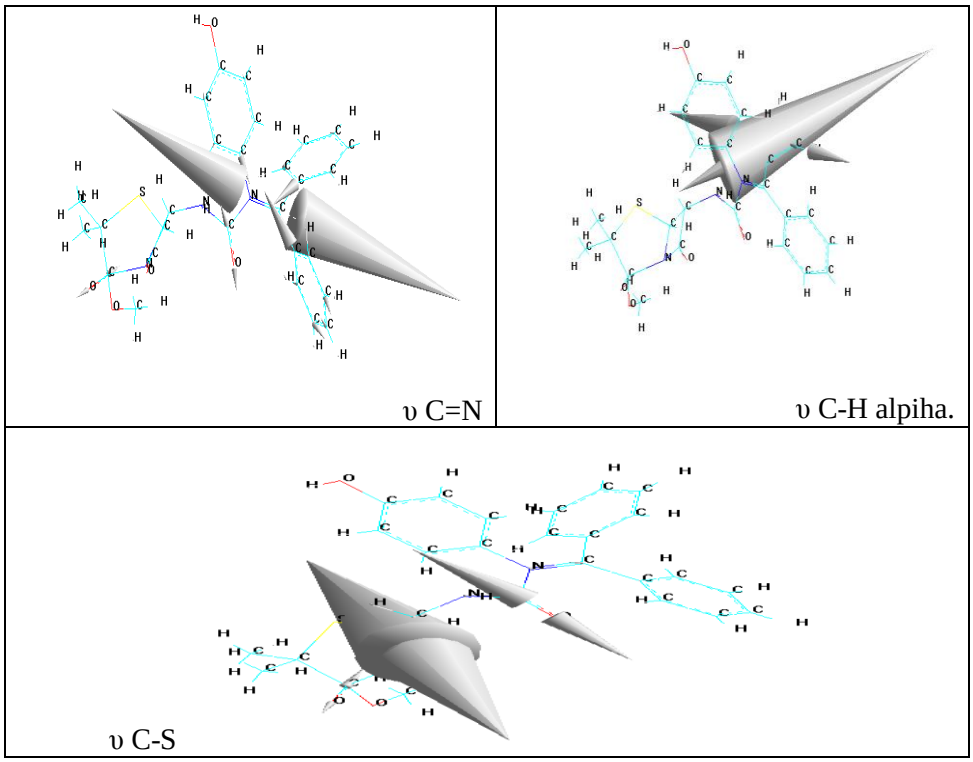

Figure 4. Vibrational frequencies of ligand

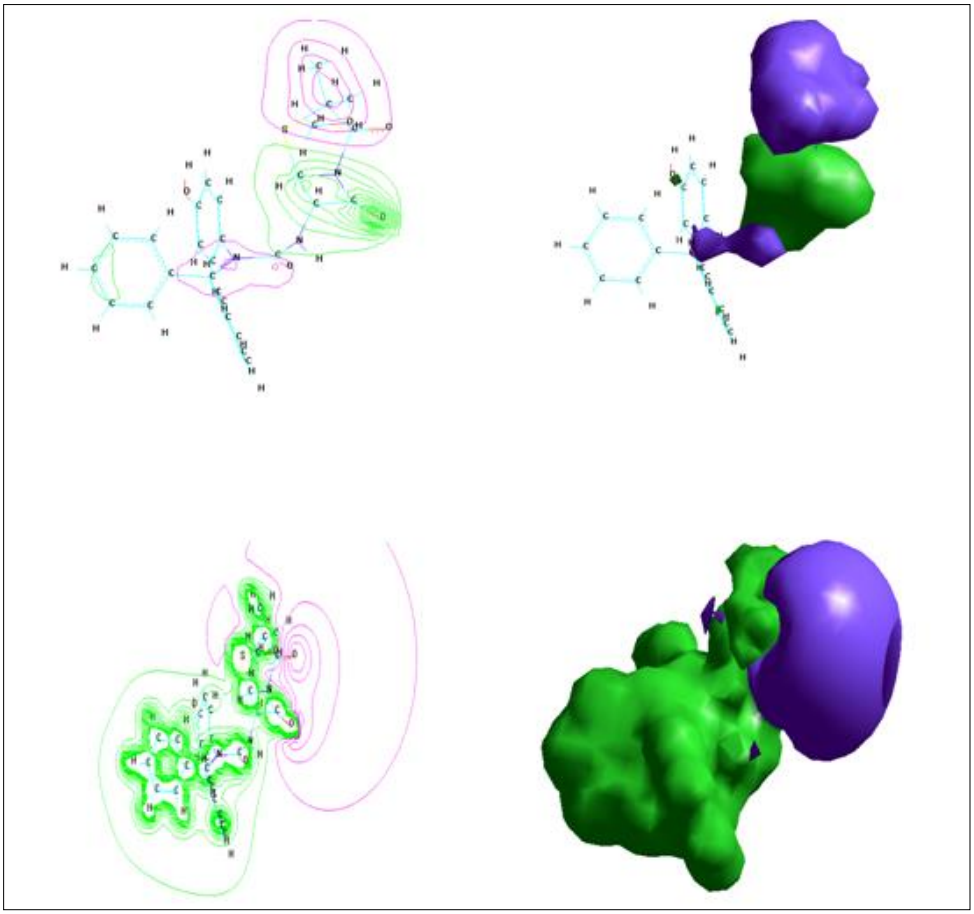

Figure 5. Electrostatic potential, HOMO & LUMO in 2,3 Dimension of Ligand

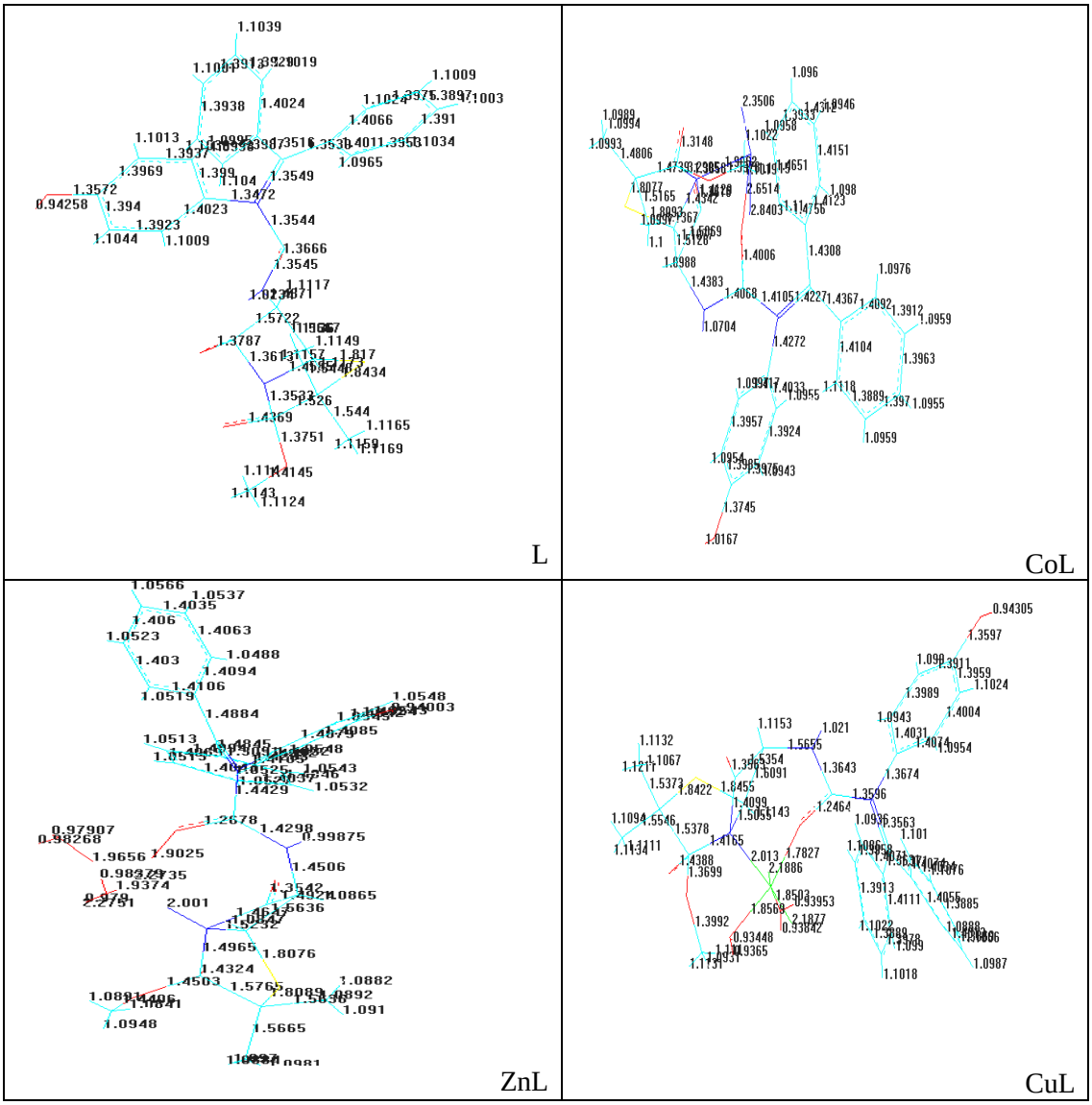

Figure 6. Bond length of prepared compounds

Conclusion:

Methyl -6-[2-(diphenylmethylene)amino)-2-(4-hydroxyphenyl)acetamido]-2,2-dimethyl-5-oxo-1-thia-4-azabicyclo[3.2.0]heptane-3-carboxylate (L) has been successfully prepared in this study. The ligand (L) has been coordinated to four diverse metal ions via oxygen and nitrogen atoms for the sake of affording the corresponding complexes. All the complexes have been two-coordinated and have presented octahedral geometry except for cobalt complex which is tetrahedral in shape. In Vitro cobalt, nickel and copper complexes have shown an inhibitory effect almost identical to that of the ligand, with the exception of the zinc complexes which showed a lower inhibition effect than other compounds.

Authors' declaration:

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are mine ours. Besides, the Figures and images, which are not mine ours, have been given the permission for re-publication attached with the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee in University of Baghdad.

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تقييم بايولوجي ودراسة نظرية لليكاند ثنائي السن مشتق من الاموكسيلين مع بعض الايونات الفلزية

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[2]وزارة التربية، بغداد-العراق

الخلاصة:

في هذا البحث تم تحضير معقدات قواعد شف للمركب ميثيل 6- (2- (ثنائي فينيل ميثيلين) أمينو) -2- (4-هيدروكسي فينيل) أسيتاميدو) -2،2-ثنائي ميثيل -5-أوكسو -1-ثيا-4-أزاباي سايكلو(0،2،3)هبتانس -3-كاربوكسيلت مع ايونات كوبلت ،نيكل ،نحاس والزنك ثنائية التكافؤ.تم تشخيص المعقدات المحضرة بطرق مختلفة منها طيف الاشعة تحت الحمراء (FT-IR) وطيف الاشعة فوق البنفسجية-المرئية (Uv-vis) ،الحساسية المغناطيسية ،التحليل الذري للعناصر (C.H.N.S) ،الامتصاص الذري والتوصيلية المولارية. الواضح من الدراسة الطيفية ان المعقدات تمتلك تركيب احادي النوية وان الليكاند المحضر متناسق مع الايونات الفلزية بشكل ثنائي السن مع شكل ثماني السطوح باستثناء معقد الكوبلت الثنائي فانة يمتلك شكل رباعي السطوح. استخدام برنامج Hyper Chem-8.0.7 لتوقع الشكل الهندسي للمركبات جنبًا إلى جنب مع حرارة التكوين ($\Delta H f°$) ، طاقة الربط (ΔEb) ، عزم ثنائي القطب (μ) ، ترددات FT-IR في الحالة الغازية . تم فحص هذه المركبات ونشاطهاالحيوي كمضادات للجراثيم والفطريات.

الكلمات المفتاحية: الفعالية البايولوجية ، معقدات قواعد شف، قواعد شف، الدراسة النظرية