



## Synthesis, Spectroscopic Characterization, and Biological Evaluation of Some Transition Metal Complexes from C<sub>16</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>S Ligand

Sahar S. Hassan<sup>1</sup>, Sameer H. Kareem<sup>1</sup>, May Faisal Ahmed<sup>2</sup>, Sura K. Ibrahim<sup>1\*</sup>, Mahasin Alias<sup>1</sup>

<sup>1</sup> Department of Chemistry, College of Science for Women, University of Baghdad, Baghdad, Iraq.

<sup>2</sup> College of Education for Pure Science Ibn-Al-Haitham, University of Baghdad, Baghdad, Iraq.

\*Corresponding Author: Sura K. Ibrahim

### Abstract

A first series of transition metal complexes were synthesized from the ligand Methyl -6- [2-(benzyl ideneamino) -2- (4-hydroxyphenyl) acetamido]-2, 2-dimethyl -5-oxo-1-thia 4-azabicyclo [3.2.0] heptane-3-carboxylate with appropriate metal salts. The complexes were characterized by spectral methods such as FTIR, UV-Visible, and Atomic absorption as well as some physical properties, molar conductivity and magnetic moment measurements. The results showed that the proposed structures of these complexes are Octahedral, except Co<sup>II</sup> is a tetrahedral geometry. The biological activities of these complexes were studied using two types of bacteria (*Staphylococcus aureus*, *Escherichia coli*) in addition to *Candida albicans* that gave results a good activity than the free ligand.

### Introduction

In pharmacology, biological activity or pharmacology activity describes its beneficial or harmful effects of drug in living materials. When the drug is a complex chemical mixture, its activity is predicated by the active ingredient in the drug substance, but can be modified by other components.

Among the various properties of chemical, pharmaceutical biological activity plays a crucial role when it used compounds in medical applications indicates [1, 2]. Transition metals have a significant position in medical inorganic chemistry. Transition metals exhibit unlike oxidation state which can interact with a sum of negative charge molecules [3]. This movement of transition metals led to the recent development of medication depends on metals and or through to be potential contender for pharmacological and helpful applications.

The impact of the mineral ion on the living cells and tissues, hence a large number of investigations and explores to control the toxic and non-toxic concentrations of metal

ions in living organisms by changing them into metal complexes [4]. Amoxicillin antibiotics, semi synthetic penicillin's is symmetric of ampicillin, with a broad spectrum of bacterial activity against many gram positive & gram negative microorganism. Metal ions can interact with many different kinds of biomolecules including DNA, RNA, protein and lipids rendering their unique and specific bioactivities. Amoxicillin acts by inhibiting bacterial cell wall synthesis. Death results due to cell wall lyses.

Therefore AMOX useful just for actively growing and synthesizing the bacterial cell wall [5, 6]. The knowledge of the interaction between metal ions and antibiotics is for a great importance because these reactions can influence the synthesis of metal antibiotics depending on the idea of metal ion interaction with absorbed drugs, for example penicillin in human body can interact with metal ions or coordinative bounded to proteins, enzyme, amino acid, nucleic bases, nucleotides and other bio ligands [7].

Theoretical chemistry may be defined as the application of mathematical and theoretical principles to the solution of chemical problems, Types of possible prediction for molecules and reactions are Heat of formation and reaction energies, Molecular energies and structures Vibration frequencies, Electronic transitions and Magnetic shielding effect [8]. A. Hussein, et.al [9]. Studied Cu(II), Co(II), Ni(II) and Fe(III) chelates of amoxicillin (AMX) antibiotic drug proved that dentate chelate was through-NH<sub>2</sub>,-that AMX acts with mentioned metal chlorides as a tri -NH, and oxygen of carbonyl β-lactam groups.

Ammar J. Alabdali, et.al [10], studied the actions of some ligands with some metal ions according to the ligands properties as bifunctional antibacterial (two β-lactams groups) complexes were expected to be more active and sensitive against both Gram-positive and Gram-negative organisms. In this work, we are interested mainly to prepared complexes derivate of amoxicillin because amoxicillin as a better starting compound and augmentation of antibacterial activity was reported by insertion of metal ions into synthesized Schiff base.

The bio-functional activity of amoxicillin is related to lactam ring that inhibits bacterial growth by proteolysis mechanism. In order to address their therapeutic failures and serious limitations, their modular design in derived form has spurred the growth of interest and been considered as a topic of research. Most of the organic drugs used against bacterial

and viral infection contain donor atoms (N, O, S) which easily coordinate with metal ions.

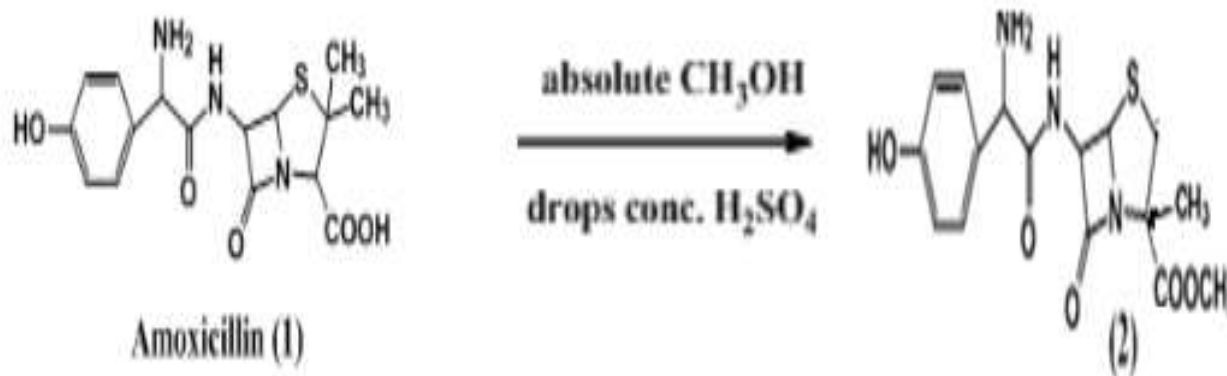
## Materials and Methods

The metal salt (CoCl<sub>2</sub>.6H<sub>2</sub>O, NiCl<sub>2</sub>.6H<sub>2</sub>O, MnCl<sub>2</sub>.6H<sub>2</sub>O, CuCl<sub>2</sub>.H<sub>2</sub>O, ZnCl<sub>2</sub>.6H<sub>2</sub>O) and (FeCl<sub>3</sub>.6H<sub>2</sub>O) in this work were obtained from Fluka, FTIR were recorded on Shimadzu 8400Fourier transform infrared spectroscopy, wavelength range of (4000-400) cm<sup>-1</sup> and UV-Vis 1600A Shimadzu was used to record the electronic spectra at wave length range of (190-1100) nm.

The metal analysis was conducted via a Perkin Elmer 500 Atomic Absorption Spectrophotometer. Conductivity Meter 220 with Gall encamps was used to calculate the molar conductivity in ethanol as a solvent at room temperature.M.F.B-6000.01 was used as a melting device. Magnetic susceptibility balance model MSB-MKT was used for magnetic moment measurement.

### Preparation of ligand C<sub>16</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>S (L)

The ligand was prepared as reported in the literature[11]6-(2-amino-2-(4-hydroxyphenyl) acetamido-2-2 dim ethyl -5-oxo-1-thia-4-azabicyclo (3.2.0) Oct -hebtane3 carboxylate .A mixture of amoxicillin (0.02mole) and an excess of absolute methanol (50ml) with (1-2) drops of concentrate sulfuric acid was placed in 100 ml round bottom flask. The mixture was refluxed in a bath water (50 °C) for 3 hrs. The solution was cooled and poured into crushed ice. The obtained precipitate was filtered, dried and recrystallized from ethanol.



### Preparation of Complexes

An amount of (CoCl<sub>2</sub>.6H<sub>2</sub>O, NiCl<sub>2</sub>.6H<sub>2</sub>O, MnCl<sub>2</sub>.6H<sub>2</sub>O, CuCl<sub>2</sub>.H<sub>2</sub>O, ZnCl<sub>2</sub>.6H<sub>2</sub>O) and FeCl<sub>3</sub>.6H<sub>2</sub>O was dissolved in 10 ml of ethanol and mixed with (ligand which

dissolved in 15 ml ethanol) in molar ratio 1:2 (M: L) in a round bottom flask under heating and refluxed for 3 hrs. The colored precipitate was filtered then washed with ethanol and dried using desiccators.

## Results and Discussion

The physio-chemical properties for the ligand and its metal complexes were summarized in Table (1). The complexes were colored powder

stable at room temperature. A molar ratio of (1:2) for the prepared complexes can be suggested according to the analytical data. The result shows all prepared complexes are electrolyte.

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

Compounds	Elemental analysis Found (cal.)				M.P C°	color	%Yield	$\mu_s \text{ cm}^{-1}$
	C	H	N	M				
$\text{C}_{16}\text{H}_{19}\text{N}_3\text{O}_3\text{S}(\text{L})$	49.04 (50)	5.26 (5.30)	18.2 (18.9)	0.00	196	Light Yellow	87	----
$\text{MnC}_{32}\text{H}_{44}\text{N}_6\text{O}_9\text{S}_2\text{Cl}_2(\text{A})$	37.11 (38.2)	4.81 (5.21)	12.4 (13.5)	4.68 (5.43)	207	light brown	80	20.9
$\text{Fe C}_{32}\text{H}_{43}\text{N}_6\text{O}_{8.5}\text{S}_2\text{Cl}_3(\text{B})$	35.21 (36.4)	4.61 (4.98)	13.21 (13.6)	4.95 (5.01)	187	Brown green	82	96.0
$\text{CoC}_{32}\text{H}_{41}\text{N}_6\text{O}_{7.5}\text{S}_2\text{Cl}_2(\text{C})$	38.67 (39.5)	4.59 (5.11)	12.35 (13.9)	5.73 (6.12)	211	Greenish blue	78	80.0
$\text{Ni C}_{32}\text{H}_{42}\text{N}_6\text{O}_8\text{S}_2\text{Cl}_2(\text{D})$	39.52 (40.5)	4.50 (4.61)	12.29 (14.01)	4.91 (5.51)	236	Greenish yellow	76	91.0
$\text{Cu C}_{32}\text{H}_{42}\text{N}_6\text{O}_8\text{S}_2\text{Cl}_2(\text{E})$	40.86 (41.60)	4.79 (5.01)	12.71 (13.63)	5.04 (5.71)	138	Green	88	62.0
$\text{Zn C}_{32}\text{H}_{42}\text{N}_6\text{O}_{7.5}\text{S}_2\text{Cl}_2(\text{F})$	39.10 (40.93)	4.26 (4.96)	13.06 (14.00)	4.34 (5.21)	201	Light yellow	87	77.0

### FT-IR Spectra of Complexes

The FTIR spectra of ligand exhibits a strong band at  $(1778) \text{ cm}^{-1}$  due to the presence of carbonyl group (C=O) of ester that appears usually around  $(1700) \text{ cm}^{-1}$ .  $\beta$ -lactam carbonyl group (C=O) occurred at a significant value about  $(1724) \text{ cm}^{-1}$ . The band of the  $\nu$  (NH) group which appears at the  $(3178.5) \text{ cm}^{-1}$ . The band at  $(1778) \text{ cm}^{-1}$  of carbonyl group of ester approximately constant in its position and did not shift in the complexes, which mean that carbonyl did not participate in coordination. The bands attributed to the  $\beta$ -lactam was shifted to higher wave number in the complexes about  $(8-15) \text{ cm}^{-1}$  indicating

that  $\beta$ -lactam carbonyl were involved in complex formation [12]. The bands of  $\nu(\text{NH})$  group were shifted to lower wave number in the complexes about  $(11-54) \text{ cm}^{-1}$  indicating that NH group was involved in complex formation. So the ligand behaves as a bidentate through the coordination via oxygen and nitrogen atoms of (C=O) and NH groups. These can be supported by the occurrence of M-O and M-N bands in the spectrum of the complexes are shown in Table (2) at the range mentioned in literatures [13, 14]. The other important characteristic peaks were observed in the FT-IR spectrum are listed in Table (2).

**Table 2: Selected IR data for Ligand (L) and its complexes**

Comp.	$\nu\text{NH}$	$\nu\text{C=O}$ Est & Amid	$\nu\text{CH}$ Alph. arom.	$\nu\text{C=O}$ $\beta$ -lactam	$\nu\text{C=C}$	$\nu\text{C-O}$	$\nu\text{M-N}$	$\nu\text{M-O}$	$\nu\text{H}_2\text{O}$
L	3032	1778 1689	2970 3151	1724	1616	1242	-	-	3444
A	3043	1778 1680	2978 3156	1732	1616	1238	536	447	3406
B	3028	1778 1680	2978 3152	1738	1616	1242	578	470	3417
C	3086	1778 1648	2974 3155	1739	1616	1230	532	415	3475
D	3055	1778 1681	2900 3186	1735	1616	1238	555	428	3410
E	3082	1778 1683	2978 3170	1739	1616	1238	567	420	3464
F	3097	1639	2947 3160	1736	1616	1246	570	451	3414

### Electronic Spectrum

The electronic absorption spectrum is used to predict the geometry according to the shape and number of observed peaks beside those

calculated once depending on the information of Racah parameter (B),  $10Dq$  and nephelauxetic factor ( $\beta$ ) using Tanabe Sugano diagram. The electronic spectrum of the

ligand shows three main bands, the first and the second absorption bands appeared at (42372 and 36363)  $\text{cm}^{-1}$  are due to (transitions located on (C=C)group. The third absorption appeared at (31250)  $\text{cm}^{-1}$  attributed to ( $\nu_1$ ) may be located on the (C=O) group [15].

### Co-Complex

The magnetic measurements showed the cobalt ion in its greenish blue complex to be paramagnetic with ( $d^7$ ) configuration in distorted tetrahedral environment [16], in infrared region the ( $\nu_1$ ) is found as a weak band at (3451) $\text{cm}^{-1}$  due to transition  ${}^4A_2 \rightarrow {}^4T_2$  [17] the ( $\nu_3$ ) was calculated as the average to three bands and assigned to the transition  ${}^4A_2 \rightarrow {}^4T_1(p)$  at about (16977)  $\text{cm}^{-1}$ , while the ( $\nu_2$ ) was calculated by reference to T.S.D for  $d^7$  configuration [18] which refer to the  ${}^4A_2 \rightarrow {}^4T_1(f)$  transition, the magnetic moment is 4.72 BM. The Racah parameter  $B'$ ,  $\beta$  and the value of (10 Dq) were also estimated as describe in Table (3).

### Ni-Complex

The electronic spectrum, show two band at (16260) and (23419)  $\text{cm}^{-1}$  for the  ${}^3A_2g \rightarrow {}^3T_1g(f)$  and  ${}^3A_2g \rightarrow {}^3T_1g(p)$  transition respectively. The transition ( $\nu_1$ )  ${}^3A_2g \rightarrow {}^3T_2g$  was calculated and it is found to be (8499)  $\text{cm}^{-1}$  other ligand filed parameter was calculated as shown in Table (3) from these data for the bands indicate Octahedral structure suggested around Ni (II) ion [19]. The magnetic moment is 3.1 BM.

### Mn-Complex

In this study, the light brown color of Mn (II) complex displays two bands at (15873) and (27027)  $\text{cm}^{-1}$  and the spectra assignments are obtained by fitting the observed spectra to Tanabsugao diagram for ( $d^5$ ) configuration. Table (3) shows the values of  $\nu_1$ ,  $B'$ ,  $\beta$  and (10Dq) computed there form [20]. Two observations have to be pointed out: (I) a series of some very weak and narrow bands has been observed in manganese spectrum. This is expected because only sextet term of

the ( $d^5$ ) configuration in Octahedral stereochemistry is the  ${}^6A_{1g}$  consequently, there can be forbidden transition [16, 18]. Furthermore, the energies of the  ${}^4E_g(G) + {}^4A_{1g}$  term do not change much relative to the  ${}^6A_{1g}$  ground terms as 10Dq change, as seen from the T.S.D therefore, bands corresponding to the transition between the ground term and these two terms are not appreciably broadened by vibronic coupling. (II) The value of the nephelauxetic ratio  $\beta$  is evaluated as the ratio of term separation complex. The electronic spectrum coupled with magnetic (3.21) BM supports the suggested octahedral geometry of this complex [19, 20].

### Fe-Complex

The electronic spectrum shows two bands at (16025) and (26315)  $\text{cm}^{-1}$  for the  ${}^6A_{1g} \rightarrow {}^4T_{2g}$  and  ${}^6A_{1g} \rightarrow {}^4A_{1g} + {}^4E_g$  transitions respectively the first transition  ${}^6A_{1g} \rightarrow {}^4T_{1g}$  calculated by using T.S.D and it is found to be (14778)  $\text{cm}^{-1}$  these band indicate Octahedral structure proposed around Fe (III) [20] the magnetic moment is 5.23 BM.

### Cu-Complex

Electronic spectrum of green displayed band at (11235)  $\text{cm}^{-1}$  which is assigned to  ${}^2E_g \rightarrow {}^2T_{2g}$  transition, the broadness of the band is due to the ligand filed and the Jan-teller effect, this absorption prefers the distortion Octahedral geometry (21). Moreover, the magnetic moment is (1.62) BM, this value lies within the expected for one electron of mononuclear Octahedral [22].

### Zn-Complex

Generally zinc ion complex with ( $d^{10}$ ) electronic configuration do not expected show (d-d) electronic transition because of the filled (d) orbital [23, 24] this complex did not show clear band in the visible region, only ILCT ligand filed bands can recognized in spectra the magnetic moment is 0.00 BM. From the data the proposed structure for the prepared complexes can be shown in Figure (1).

**Table 3: The electronic spectra and their assignment of the prepared complexes**

Comp.	Band $\text{cm}^{-1}$	Assignment	$B' \text{cm}^{-1}$	Dq/B'	B	10Dq $\text{cm}^{-1}$
L	67613	$\pi-\pi^*$	-----	-----	-----	-----
	42372					
	31250					

		n- $\pi^*$				
A	12951(cal.) 15873 27027	${}^6A_{1g} \rightarrow {}^4T_{1g}$ ${}^6A_{1g} \rightarrow {}^4T_{2g}$ ${}^6A_{1g} \rightarrow {}^4A_{1g}+{}^4E_g$	860	1.78	0.84	1295
B	14778 16025 26315	${}^6A_{1g} \rightarrow {}^4T_{1g}$ ${}^6A_{1g} \rightarrow {}^4T_{2g}$ ${}^6A_{1g} \rightarrow {}^4A_{1g}+{}^4E_g$	1300	1.82	0.62	1477
C	3451 5217(cal.) 16977	${}^4A_2 \rightarrow {}^4T_2$ ${}^4A_2 \rightarrow {}^4T_2(F)$ ${}^4A_2 \rightarrow {}^4T_1(p)$	970	0.47	0.76	3470
D	8499 16260 23419	${}^3A_{2g} \rightarrow {}^3T_{2g}$ ${}^3A_{2g} \rightarrow {}^3T_{1g}(F)$ ${}^3A_{2g} \rightarrow {}^3T_{1g}(p)$	1035	1.2	0.68	8499
E	11235 26595 24691	${}^2E_g \rightarrow {}^2T_{2g}$ C.T charge transfer C.T charge transfer	-	-	-	-
F	4926 31347	$\pi-\pi^*$ C.T Charge transfer	-	-	-	-

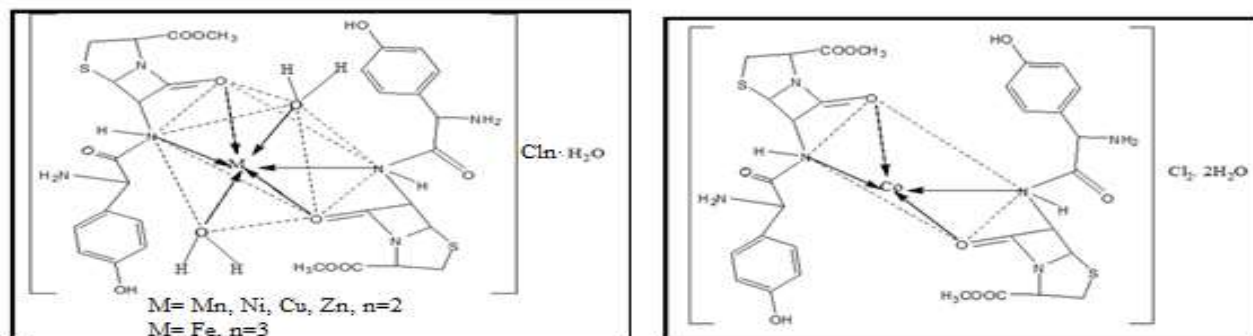


Figure 1: The Proposed structure for the prepared complexes

## Theoretical Study

### Optimized Geometries and Energies

The program HyperChem-8.07 is used for the semi-empirical calculation at optimized geometries energies [25].

The results of PM<sub>3</sub> methods of calculation in gas phase for heat of formation ( $\Delta H_f^\circ$ ), binding energy ( $\Delta E_b$ ) and total energy ( $\Delta E_T$ ) for the ligand and its complexes are calculated and tabulated in (Table 4).

Table4: Conformation Energetic (in KJ.mol<sup>-1</sup>) for the Ligand and its Metal Complexes

Compound	PM3		
	$\Delta H_f^\circ$	$\Delta E_b$	$\Delta E_T$
L	-590.316	-4843.556	-103278.258
L-Cu	-1820.989	-42443.263	-1038341.355
L-Fe	-2913.256	-43613.350	-975882.172
L-Mn	-1859.419	-42427.299	-961678.450
L-Ni	-2400.017	-43114.756	-1024743.836
L-Zn	-1253.798	-41668.836	-926371.289
L-Co	-2260.447	-41603.143	-937810.061

### Optimized vibrational Spectra for (L)

Theoretically calculated wave numbers for the ligand show some deviations from the

experimental values [26]. These deviations are generally acceptable in theoretical calculation [27] and are described in (Table 5).

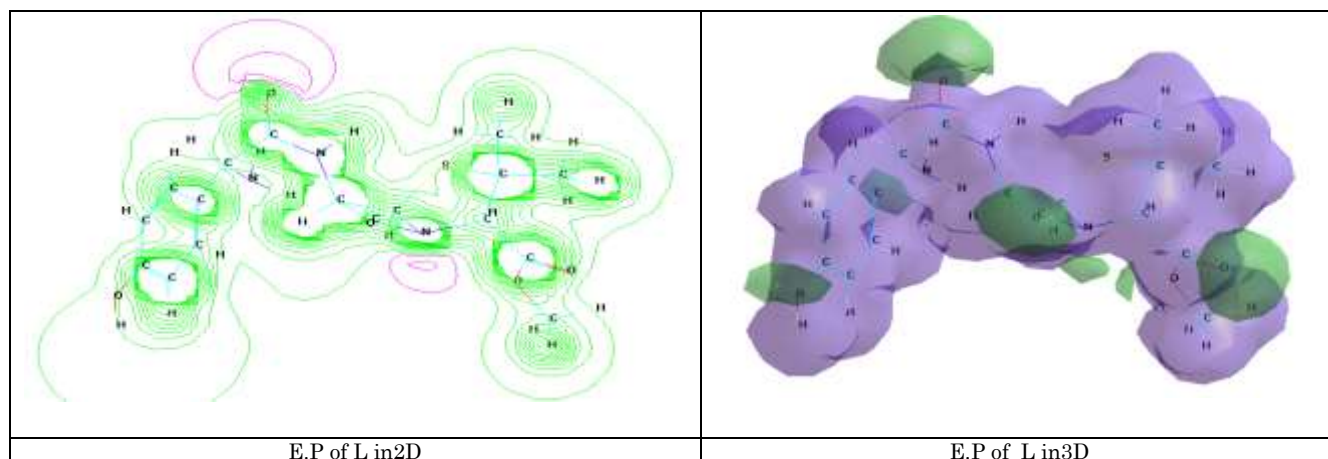
**Table 5: A Comparison between Experimental and Theoretical Vibrational Frequencies for the Ligand (cm<sup>-1</sup>)**

Compound	$\nu$ NH <sub>2</sub>	$\nu$ N-H Amide	$\nu$ C-H Aliph. Asym. Sym.	$\nu$ C-H Arom.	$\nu$ C=C Arom	$\nu$ C-O	$\nu$ C-N	$\nu$ C-S
L	3526	3169	2970	3042	1584	1251	1367	1179
	3517*	3325*	3073*	3061*	1562*	1353*	1439*	1174*
	-0.255**	4.922**	3.468**	0.624**	-1.388	8.153**	5.267**	-0.0424**
			2936		1518			
			2944*		1477*			
			0.272**		-2.700**			

Experimental frequencies

\*Theoretical frequencies

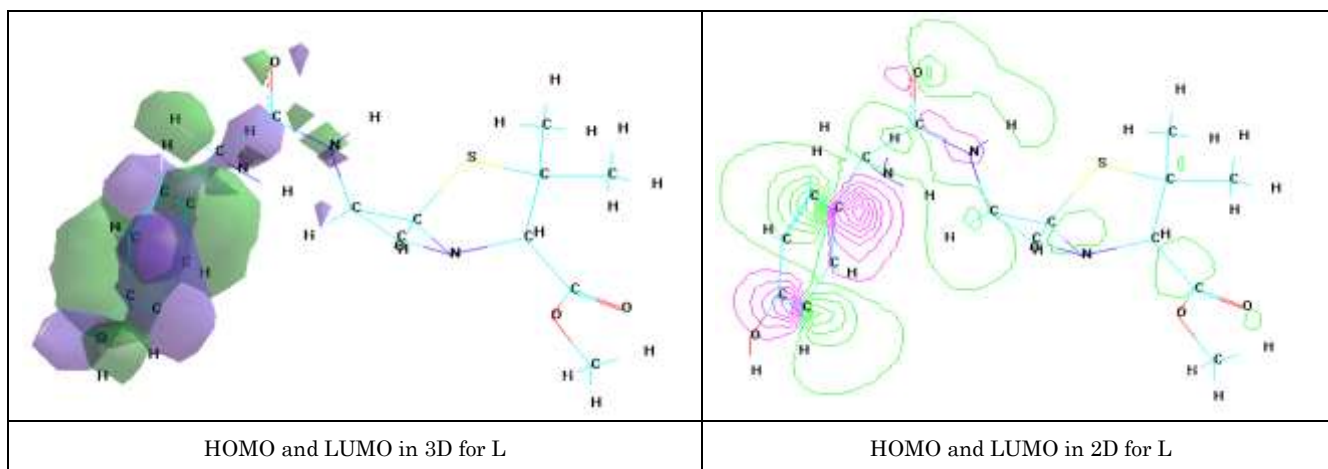
\*\*Error %

**Figure 2: Electrostatic Potential as 2D&3D Counters for L**

### Electrostatic Potential

It designates the interaction of energy of the molecular system with a positive charge point that is the reason why it is practical for finding sites of reaction in molecule positive charge species. They tend to attack a molecule wherever the E.P is powerfully negative electrophonic attach. The E.P of the

free ligand is measured and plotted as 2D and 3D contour to inspect the reactive sites of the molecules shown in Figure(2). The results of calculation illustrate that the LUMO of transition metal ion choose to react with the HOMO of donor atoms in ligand [28, 29], as shown in Figure (3) via adopting Hyperchem.-8.07 program.

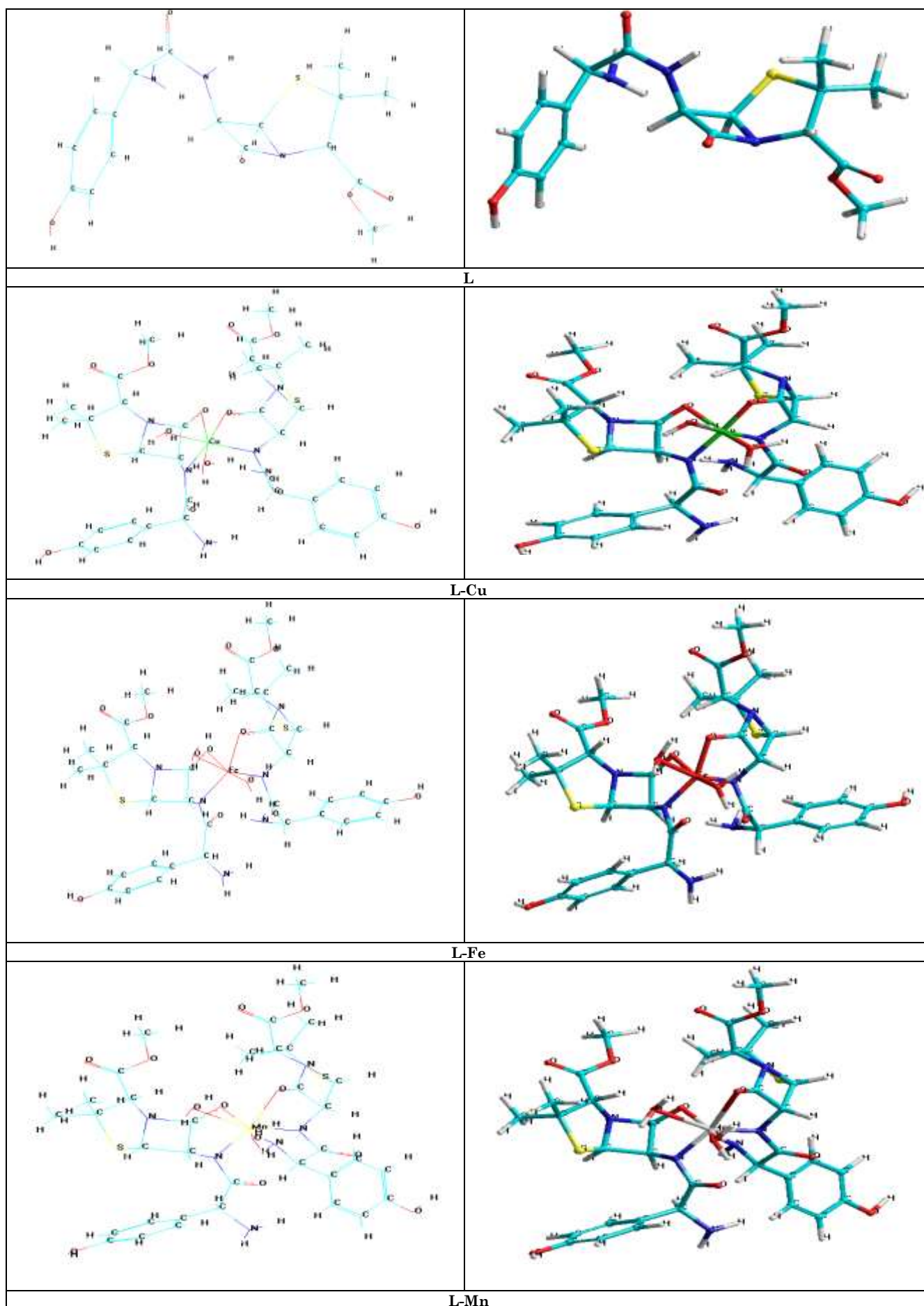
**Figure 3: HOMO and LUMO Sites for the L**

### Optimized Geometries and Energy of Metal Complexes for the Ligand

Theoretically probable structures of metal complexes with ligand have been calculated to find the most possible model building

stable structure. The shapes appearing in Figure (4) indicate the calculation optima geometries for the ligand and its complexes. The outcomes of PM3 method of calculation in gas phase for  $\Delta H^{\circ}_f$ ,  $\Delta E_b$  and  $\Delta E_T$  are

tabulated in Table (1) for L, Fe(II), Ni(II), Cu(II), Co(II), Mn(II) and Zn (II) complexes.



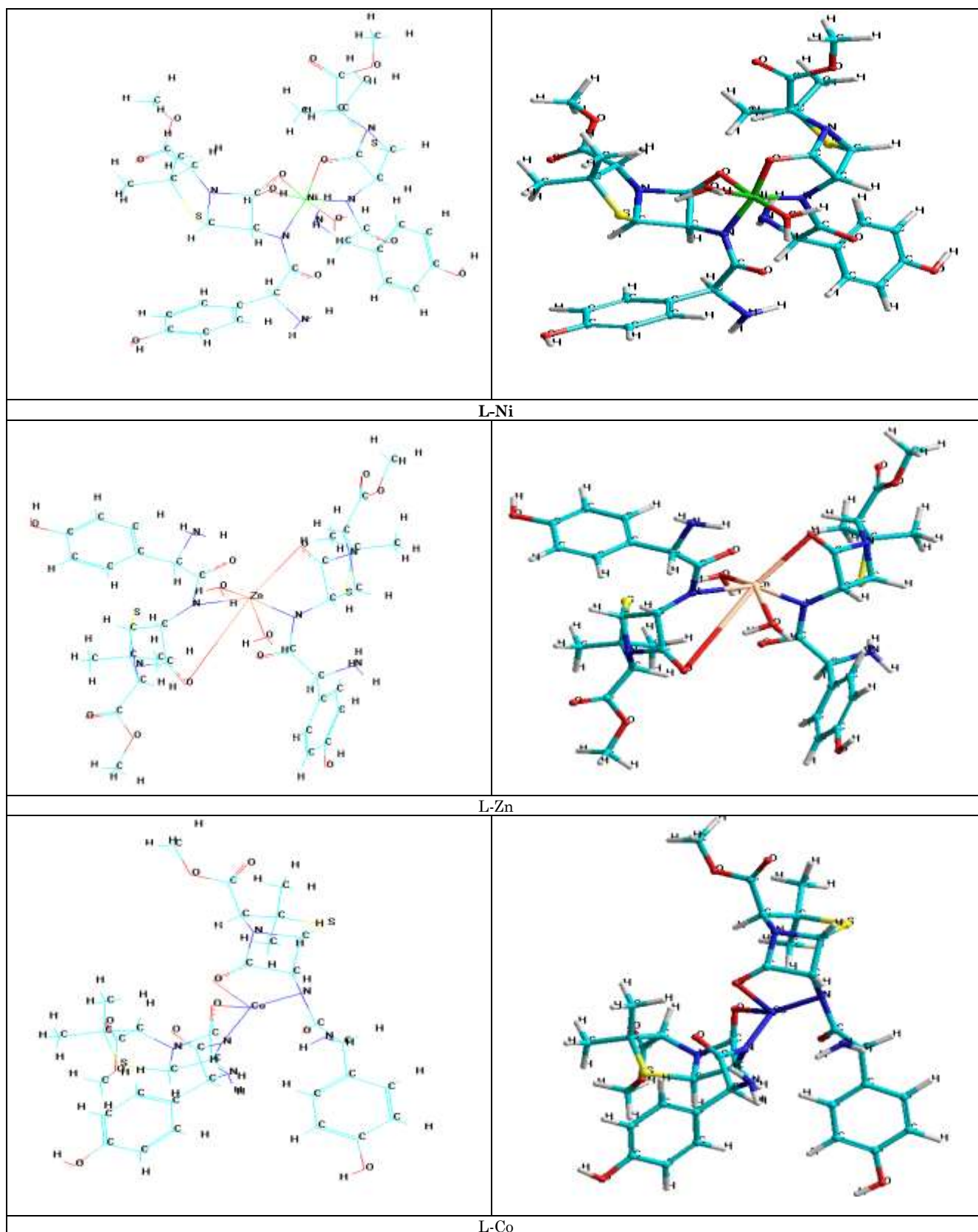


Figure 4: Conformation Structure of Ligand and its Metal Complexes Using Hyperchem-.8.7. Program

### Antibacterial Activities

The microorganisms have the ability to develop resistance to these chemotherapeutic agents and such strains which are resistant causing major problem in treatment of microbial infections. Searching for new antimicrobial agents become something very necessary, therefore a great effort have been employed to find new antibiotics or new

compounds with good antimicrobial activity which might be suitable to be used as chemotherapeutic agents [30].

In this study ,the synthesized complexes were evaluated for their *in-vitro* antimicrobial activity against some of the pathogenic bacteria, four bacterial species were used Gram positive *staphylococcus*



*aures*, *Bacillus subtilis* Gram negative bacteria *Pseudomonas aeruginosa*, *Escherichia coli* used the concentration ( $10^{-3}$ ) M for all compounds. The data of antimicrobial activities of the prepared ligand and its metal complexes are given in Table (6). The cobalt (II) and Nickel (II) complexes show higher inhibition against both organisms effect compared with free ligand. The iron (III) and manganese (II) complexes showed moderate activate and the Zinc (II), Copper (II) complexes show a non-activity respectively. The higher inhibition zone of metal complexes than the ligand can be explained on the basis of chelation theory and overtone concept [31,32].

One chelation, the polarity of the metal ion will be reduced eater extent due to the overlap of the ligand orbital and partial.

Sharing of the positive charge of the metal in the donor groups. Further, it increases the delocalization of the-electrons over the whole chelating ring and enhances. The penetration of the complexes in the lipid membranes and blocking of the metal binding sites in the enzyme of microorganisms.

These and other factors which also increase the activity are the solubility, conductivity ,geometry ,and bond length between the metal and the ligand [32,33] as shown in Figures (5, 6, 7 and 8).

**Table 6:** Show The effect of ligand and its metal complexes toward *staphylococcus aures*, *Bacillus subtilis* *Pseudomonas aeruginosa*, *Escherichia*

Bacteria	CuL (1)	FeL (2)	ZnL (3)	L (4)	MnL (5)	NiL (6)	CoL (7)
<i>Staphylococcus aureus</i>	+	++	+	++	+	+++	+++
<i>Bacillus subtilis</i>	+	+	-	++	++	++	+++
<i>Escherichia coil</i>	-	+	+	++	+	+	++
<i>Pseudomonas aeruginosa</i>	-	+	-	+	+	+	+

(-) No signification.

(+) Slight signification zone of which (5-10mm)

(++) Moderated significant zone of which (11-20mm)

(+++) High significant zone of which (>20)



**Figure 5:** The effect of compound on *Bacillus subtilis*



**Figure 6:** The effect of compounds on *Staphylococcus aureus*



**Figure 7:** The effect of compounds on *Pseudomonas aeruginosa*

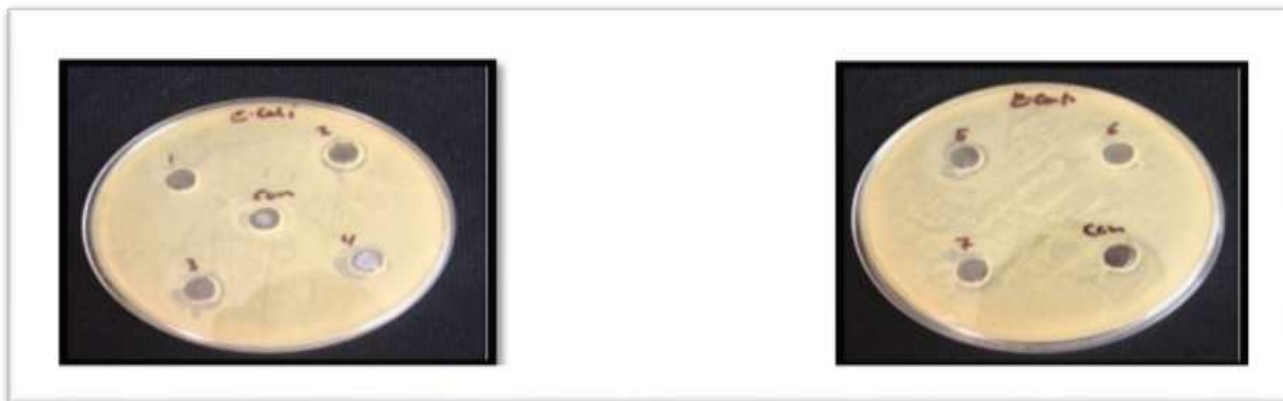


Figure 8: The effect of compounds on *Escherichia coli*

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