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## Complexes of Some Transition Metal with 2-Benzoyl thiobenzimidazole and 1,10-Phenanthroline and Studying their Antibacterial Activity

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### Abstract:

Mixed ligands of 2-benzoyl Thiobenzimidazole ( $L_1$ ) with 1,10-phenanthroline ( $L_2$ ) complexes of Cr(III), Ni(II) and Cu(II) ions were prepared. The ligand and the complexes were isolated and characterized in solid state by using FT-IR, UV-Vis spectroscopy,  $^1\text{H}$ ,  $^{13}\text{C}$ -NMR, flame atomic absorption, elemental micro analysis C.H.N.S, magnetic susceptibility, melting points and conductivity measurements. 2-Benzoyl thiobenzimidazole behaves as bidentate through oxygen atom of carbonyl group and nitrogen atom of imine group. From the analyses Octahedral geometry was suggested for all prepared complexes. A theoretical treatment of ligands and their metal complexes in gas phase were studied using HyperChem-8 program, moreover, ligands in gas phase also has been studied using Gaussian program (GaussView Currently Available Version (5.0.9) along with Gaussian 09 which was the latest in the Gaussian series of programs). The antibacterial activity of the prepared complexes have been determined and compared with that of the ligand and the standard metronidazole.

**Key words:** Mixed ligands, 1,10-Phenanthroline, Theoretical treatment, Antibacterial activity.

### Introduction:

The interaction of heterocyclic thiones with metals is still the topic of several studies as these ligands contain chemically effective groups and are advantageous model compounds for sulfur containing analogues of purine and pyrimidine bases. Heterocyclic 2-thiones bind to a metal in different

ways, leading to the formation of monomeric or polymeric complexes [1]. Mercapto-1,3-azole ligands play an important role in industry and medicine [2,3]. One of their attractive characters is their acidity, which could affect their chemical reactivity toward transition metal ions and determine the complexes final structure [4].

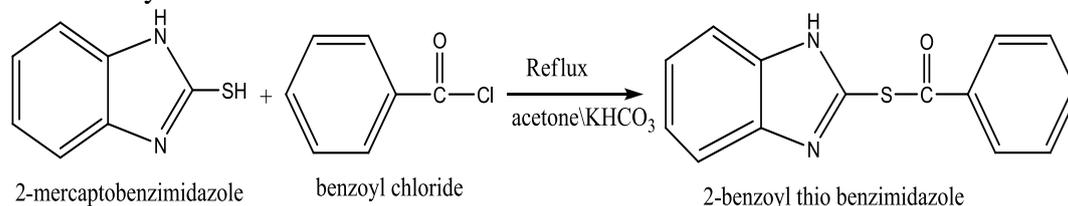
1,10-phenanthroline has been extensively used as ligand, due to their high chemical stability and their good coordination ability. This ligand coordinate easily to metal ions forming a stable ring with five atoms [5]. Metal complexes of phenanthroline chelators are of great interest since they exhibit numerous biological properties such as antitumor and antibacterial activity [6,7]

Mixed ligand complexes plays an important role in numerous chemical and biological systems like water softening, ion exchange resin, electroplating, dyeing, antioxidant, photosynthesis in plants, removal of undesirable and harmful metals from living organisms. Many of these metal complexes shown good biological activity against pathogenic microorganisms[8,9]. In this study has been devoted to prepared and characterize the mixing ligands and their metal complexes. In vitro antibacterial activity of all prepared compounds have also been performed.

## Materials and Methods:

### A- Instrumentation:

All chemicals and solvents used and were of highest purity obtained from Fulka, Merck and BDH. Melting point apparatus of Gallen Kamp M.F.B-60 was employed to gauge the prepared compounds melting points, Elemental CHNS analysis were carried out on a



**Scheme(1): Preparation of 2-benzoyl Thiobenzimidazole**

### 2- Preparation of complexes by conventional method

A Solution containing primary ligand 2-benzoyl Thiobenzimidazole (0.254gm, 1mmole) and secondary ligand 1,10-phenanthroline (0.198gm, 1mmole) each dissolved in 5 ml of absolute ethanol

EM-017.mth instrument, the FT-IR spectra were recorded in range (4000-200  $\text{cm}^{-1}$ ) as CsI disc on IR-Prestige-21, Single beam path Laser, Shimadzu Fourier Transform infrared Spectrophotometer, UV-Visible spectra were measured using UV-1800PC Shimadzu, in the range (190-1100) nm. The  $^1\text{H}$ ,  $^{13}\text{C}$ -NMR spectra were recorded on Burker 400MHz instrument using DMSO- $\text{d}_6$  as solvent and TMS as internal reference in AL-Bayt University, Jordan. The magnetic susceptibility values of the prepared complexes were carried out in room temperature using Magnetic Susceptibility Balance of Johanson mattey catalytic system division. Atomic absorption measurements of the prepared complexes were obtained using Shimadzu Atomic Absorption 680 Flame Spectrophotometer. The conductance values of the prepared complexes were preformed using 0.001M Ethanol as a solvent, (WTW) Conductometer. The conventional method were used to prepare metal complexes.

### B- Synthesis of compounds

#### 1- Preparation of 2-benzoyl Thiobenzimidazole

According to the literature [10], The ligand 2-benzoyl Thiobenzimidazole prepared as in the following scheme :

was added to a warm solution of metal salts (1mmole) of  $[\text{CrCl}_3 \cdot 6\text{H}_2\text{O}]$  (0.26g);  $[\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}]$  (0.29g);  $[\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}]$  (0.24g), in 10 ml of absolute ethanol. The mixture was heated and refluxed with stirring for (3-4) hrs. The colored products was filtered, washed several

times with ethanol, and dried using the electrical oven at (65°C).

### Results and Discussion:

The physio-chemical properties of the complexes are tabulated in Table (1).

The isolated solid complexes are stable at room temperature and soluble in Ethanol and most organic solvents. The spectroscopy and magnetic studies were used to confirm their formation and suggested geometry, (Tables 2 and 3).

**Table (1): Some analytical and physical data of the ligands and their metal complexes.**

Compd. Colour	Yield %	M. p. °C	M. Wt g.mol <sup>-1</sup>	% Elemental micro analysis / Found (Calc.)				Metal% Found (Calc.)
				C	H	N	S	
C <sub>14</sub> H <sub>10</sub> N <sub>2</sub> SO(L1) Light yellow	86	169-171	254.00	67.01 (66.14)	4.22 (3.93)	11.53 (11.02)	13.02 (12.59)	-----
C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> .H <sub>2</sub> O(L2) White	----	100-102	198.00	(72.72)	(5.05)	(14.14)	----	-----
[CrL <sub>1</sub> L <sub>2</sub> Cl <sub>2</sub> ]Cl.2H <sub>2</sub> O Green	72.70	146-148	646.49	48.29 (48.26)	3.86 (3.71)	8.68 (8.66)	4.95 (4.94)	7.99 (8.04)
[NiL <sub>1</sub> L <sub>2</sub> OH <sub>2</sub> (ONO <sub>2</sub> )]NO <sub>3</sub> .3H <sub>2</sub> O Green	83.25	180-182	706.69	44.03 (44.14)	3.10 (3.67)	11.77 (11.88)	4.44 (4.52)	7.97 (8.30)
[CuL <sub>1</sub> L <sub>2</sub> OH <sub>2</sub> (ONO <sub>2</sub> )]NO <sub>3</sub> .1/2H <sub>2</sub> O Dark Blue	84.37	150-152	666.54	47.45 (46.80)	3.43 (3.45)	12.68 (12.60)	4.68 (4.80)	10.00 (9.53)

### FT-IR Spectra:

The most important infrared bands for the ligands and their complexes are reported in Table (2). The most important bands appeared in the spectrum of ligand L<sub>1</sub>, appeared at (1705; 1620; 784; and 1176 cm<sup>-1</sup>) which assigned to stretch frequency of  $\nu(\text{C}=\text{O})$ ;  $\nu(\text{C}=\text{N})$ ;  $\nu(\text{CS})$ ; and  $\nu(\text{CSC})$  respectively [11].

The spectra of metal complexes show that the band related to stretch frequency of  $\nu(\text{C}=\text{O})$  was shifted to the lower or higher frequencies about (12 to 20cm<sup>-1</sup>) in complexes, which indicate that the uncharged oxygen of carbonyl group take part in the coordination[11], more evidences new weak bands appeared in the spectra of complexes at lower frequencies about (~ 462-489 cm<sup>-1</sup>) which assigned to  $\nu(\text{M}-\text{O})$  bond[15]. Also the band related to the stretching frequency of  $\nu(\text{C}=\text{N})$  was shifted to the lower frequency in CrL<sub>1</sub>L<sub>2</sub> about (9 cm<sup>-1</sup>) and to the higher in CuL<sub>1</sub>L<sub>2</sub> and NiL<sub>1</sub>L<sub>2</sub> frequencies about (~7-8cm<sup>-1</sup>). This means that the nitrogen of (C=N) group also coordinated with metal ion, a new weak bands were recorded at lower frequencies by (~563-570 cm<sup>-1</sup>) which assigned to

stretch frequency of  $\nu(\text{M}-\text{N})$  bond was supported this coordinate[11,12]. So, this ligand behaves as a bidentate through (cyclic N and O) atoms. Higher shifting frequencies related to the amide(II) in metal complexes, also  $\nu(\text{NH})$  group shift to higher in among L<sub>1</sub> complexes due to the possible hydrogen bonding interaction between (C=O) and (N-H) moiety[11]. The presence of peaks that attributed to the aromatic C=C and C=N stretching of L<sub>2</sub> around (1616-1419cm<sup>-1</sup>) [11], so the spectra of the complexes show also characteristic bands which shifted and assigned to the stretching vibration of  $\nu(\text{C}=\text{C}+\text{C}=\text{N})$  of co-ligand. The band at (400 cm<sup>-1</sup>) related to (C-C out of plane bending) shifts to higher frequency and splits into two components in the complexes, which again confirms the coordination of co-ligand through two nitrogen, besides it shows bands at (~ 271-288 cm<sup>-1</sup>) has also been observed in all the complexes indicating co-ligand nitrogen coordination with metal ions as (M-N)[12]. The spectrum of CuL<sub>1</sub>L<sub>2</sub> and NiL<sub>1</sub>L<sub>2</sub> exhibited bands which appeared at 1018, 1292, 1381 and 1427 cm<sup>-1</sup>; 783, 1041, 1234 and 1373cm<sup>-1</sup> respectively, probably attributed to the vibrations of

ionic and non-ionic nitrate group[11]. CrL<sub>1</sub>L<sub>2</sub> complex was observed band at 312 cm<sup>-1</sup> due to the coordination of metal ion with chloride ions[11]. A

broad band with maximum (3352-3448 cm<sup>-1</sup>) which assigned to lattice water as well as coordinated in coordination sphere.

**Table (2):The most diagnostic FTIR of the ligands and their metal complexes in (cm<sup>-1</sup>).**

Compd.	L <sub>1</sub>	L <sub>2</sub>	[Cr L <sub>1</sub> L <sub>2</sub> Cl <sub>2</sub> ]Cl.2H <sub>2</sub> O	[Ni L <sub>1</sub> L <sub>2</sub> (OH <sub>2</sub> )(ONO <sub>2</sub> )]NO <sub>3</sub> .3H <sub>2</sub> O	[CuL <sub>1</sub> L <sub>2</sub> (OH <sub>2</sub> )(ONO <sub>2</sub> )]NO <sub>3</sub> .1/2 H <sub>2</sub> O
v(N-H)	3151	-----	3140	3155	3150
v(C=O)	1705	-----	1717	1689	1685
v(C=N)	1620	-----	1611	1628	1627
v(C=C)	1504	-----	1500	1516	1500
vC-H arom.	3059	3059	3059	3080	3070
δ(C-H) <sub>oop</sub>	783,883,848	802,731	883,848,806,783	883,848,825	875,848,823,802
δ(C-H) <sub>ip</sub>	1234,1284,1176,1130	1265,1202,1164,1138,1033	1284,1253,1234,1219,1199,1176,1103	1262,1234,1210,1200,1172,1145,1103	1292,1226,1203,1167,1149,1103
v(CSC)	1176	-----	1199	1172	1149
v(CS)	748	-----	752	752	750
v(C=N+ C=C)	-----	1616,1589,1558,1504,1446,1419	1611,1600,1578,1500,1470,1450,1423	1628,1600,1585,1516,1450,1427	1619,1585,1500,1458,1427
v(M-N)	-----	-----	565	570	563
v(M-O)	-----	-----	486	474	462
v(M-N) <sub>Phen</sub>	-----	-----	288	273	271
Others	-----	vH <sub>2</sub> O= 3410,3383	vH <sub>2</sub> O = 3398	vH <sub>2</sub> O = 3352 NO <sub>3</sub> = 783,1041,1234,1373	H <sub>2</sub> O = 3448 NO <sub>3</sub> = 1018,1292,1381,1427

Where oop= out of plane , ip= in plane

Phen. = Phenanthroline

### Electronic spectral, Magnetic moment studies and Conductivity:

The electronic spectrum of L<sub>1</sub> exhibited four main bands. The first and second absorption bands appeared at (45871, 40485 cm<sup>-1</sup>) respectively due to (π→π\*) transition located on the C=C group. The third and fourth absorption bands attributed to (n→π\*) electronic transition may be located on the Nitrogen atom of the -C=N-group or Oxygen on C=O group, which appeared at (32786,29239 cm<sup>-1</sup>) respectively [10,13,14] as listed in Table (3).

The electronic Spectrum of co-ligand L<sub>2</sub> show absorption band in the ultraviolet region at (43859 cm<sup>-1</sup>) due to the (π→π\*) transition for the inter-ligand aromatic system (C=C), and other absorption bands at (30959 and 38022) due to the (n→π\*) transition of imine group (C=N) [13].

Cr(III) Complex: The spectrum of green Cr(III) consists of two bands observed at 17006 , 24390 cm<sup>-1</sup> refers to <sup>4</sup>A<sub>2g</sub>→<sup>4</sup>T<sub>2g</sub> , <sup>4</sup>A<sub>2g</sub>→<sup>4</sup>T<sub>1g(F)</sub> transitions[15].The ν<sub>3</sub> band calculated to be 38379 cm<sup>-1</sup> which corresponding to <sup>4</sup>A<sub>2g</sub>→<sup>4</sup>T<sub>1g(p)</sub> transition. The magnetic value 3.92 B.M. for Chromium (III) is observed, this value came in with published octahedral geometry around Cr(III) ion[16,17].

Ni(II) Complex: The electronic spectrum, shows two bands at 11001, 16233cm<sup>-1</sup> which assigned to <sup>3</sup>A<sub>2g</sub>→<sup>3</sup>T<sub>2g</sub> , <sup>3</sup>A<sub>2g</sub>→<sup>3</sup>T<sub>1g(F)</sub> respectively and <sup>3</sup>A<sub>2g</sub>→<sup>3</sup>T<sub>1g(p)</sub> transitions calculated and its found to be 27855 cm<sup>-1</sup>. These bands indicate an octahedral geometry around Ni(II) ion [18]. Magnetic measurement show to be 3.02 B.M and this came with published Oh around Ni(II)[15,19].

The diagrams of Tanabe–Sugano used to estimate the value of  $v_3$  in the complexes of Cr(III) and Ni(II) ions. In addition to the calculation of values;  $10Dq$ , nephelauxetic factor  $\beta$ , Racah parameter  $B'$  and  $15B'$  Table (3).

**Cu(II) Complex:** The electronic spectrum, show broad absorption band at  $14814 \text{ cm}^{-1}$  which assigned to  ${}^2E_g \rightarrow {}^2T_{2g}$  and other bands at  $36630, 43478 \text{ cm}^{-1}$  which related to charge transfer transitions. Magnetic measurement showed to be 1.85 B.M and this came with published Octahedral around Cu(II)[20].

The conductance measurements indicate that the ionic behavior for all prepared complexes as illustrated in Table (3).

#### NMR spectra for ligand

#### ${}^1\text{H-NMR}$ spectrum

${}^1\text{H-NMR}$  spectrum for ligand by using DMSO solvent showed band at the range (2.415-2.511)ppm which due to the protons of solvent and multiple bands appear at the range (7.185-7.839) ppm return to the aromatic ring protons while the NH Group showed one band at the position (12.55) ppm.

#### ${}^{13}\text{C-NMR}$ spectrum

${}^{13}\text{C-NMR}$  spectrum for ligand by using DMSO solvent showed multi bands at the range (38.63-43.79)ppm which return to the carbon of the following groups 2C-S, 1C=N, 1C-N and multi bands appear at the range (122.27-134.98) ppm assigned to the aromatic ring carbons while the carbonyl group showed four bands at the range (168.71-169.84) ppm.

**Table (3): Electronic spectra, Conductance in Ethanol solvent and magnetic moment (B.M) for the ligands and their metal complexes.**

Compd.	$L_1$	$L_2$	$[\text{Cr } L_1L_2Cl_2]Cl \cdot 2H_2O$	$[\text{Ni } L_1L_2OH_2ONO_2] NO_3 \cdot 3H_2O$	$[\text{Cu } L_1L_2OH_2ONO_2] NO_3 \cdot 1/2H_2O$
<b>Absorption Bands <math>cm^{-1}</math> (nm)</b>	29239(342) 32786(305) 40485(247) 45871(218)	30959(323) 38022(263) 43859(228)	17006(588) 24390(410) 38379 (260) <sub>cal.</sub>	11001(909) 16233(616) 27855(359) <sub>cal.</sub>	14814(675) 36630(273) 43478(230)
<b>Assignments</b>	$n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$	$n \rightarrow \pi^*$ $\pi \rightarrow \pi^*$	${}^4A_{2g} \rightarrow {}^4T_{2g}$ ${}^4A_{2g} \rightarrow {}^4T_{1g(F)}$ ${}^4A_{2g} \rightarrow {}^4T_{1g(P)}$	${}^3A_{2g} \rightarrow {}^3T_{2g}$ ${}^3A_{2g} \rightarrow {}^3T_{1g(F)}$ ${}^3A_{2g} \rightarrow {}^3T_{1g(P)}$	${}^2E_g \rightarrow {}^2T_{2g}$ ILCT ILCT
$B^\circ (cm^{-1})$			918	1035	
$B' (cm^{-1})$			811	739	
$B$			0.88	0.71	
$Dq/B' (cm^{-1})$			2.00	1.45	
$10Dq (cm^{-1})$			16220	10715	
$15B' (cm^{-1})$			12165	11085	
$\lambda' (cm^{-1})$				-180	
$\mu_{eff} B.M.$			3.92	3.02	1.85
$\mu_s cm^{-1}$			36.3	40.1	42.2
<b>Suggested geometry</b>			Oh	Oh	Oh

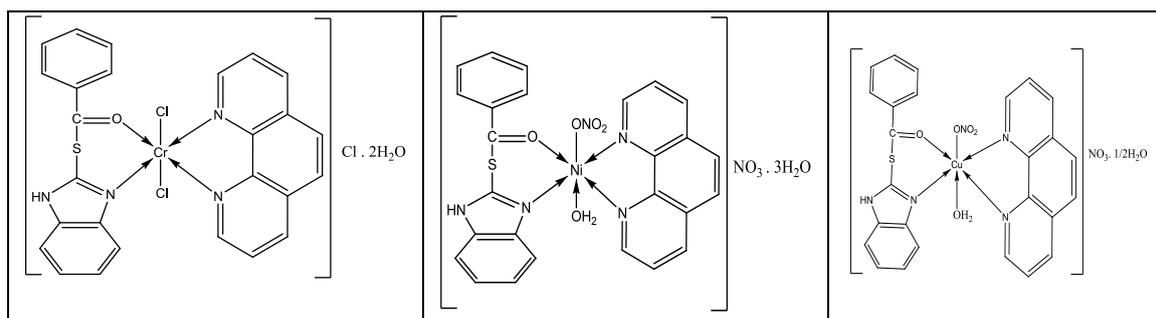


Fig. (1): Suggested structure of the prepared complexes.

### Theoretical Studies:

In this work, Hyperchem-8 program was used to calculate the heat of formation ( $\Delta H_f^\circ$ ), binding energy ( $\Delta E_b$ ) and dipole moment ( $\mu$ ) for the free ligands and their metal complexes using semi-empirical (ZINDO/I & PM3) and molecular mechanics (AMBER) methods at 298K [21]. It was found that the complexes are more stable than the ligands Table (4). Furthermore, the electrostatic potential for free ligands was calculated to investigate the reactive site of the molecules Figure (2), PM3 was used to evaluate the vibrational spectra of free ligands. It has been found that these obtained frequencies agree well with the experimental results ; in addition , the calculation helped to assign unambiguously the most diagnostic bands, Table (6,7). Electronic

spectra measurements for the ligands was calculated theoretically by using ZINDO/S method and comparing it with experimental results. It was found that there was a close agreement between the theoretical calculation and experimental results Table (8). While Gaussian program semi-empirical (PM3) method was used to calculate, the geometry optimization , dipole moment ( $\mu$ ) and total energy as shown in Table (5), electrostatic potential,  $E_{LUMO}$  and  $E_{HOMO}$  was obtained Figure (2) and evaluate the vibrational spectra by PM3 as above mentioned Table (6,7). Electronic spectra measurements for the ligands was calculated theoretically by using the job type : Single point energy (SP) along with ZINDO method and also along with CIS method (3-21G) Table (9).

Table (4): Conformation energetic (in K.J.mol<sup>-1</sup>) and dipole moment (in Debye) for ligands and their metal complexes using HyperChem-8 program.

Comp.	PM3			ZINDO/I		
	$\Delta H_f^\circ$	$\Delta E_b$	$\mu$	$\Delta H_f^\circ$	$\Delta E_b$	$\mu$
L <sub>1</sub>	303.9117786	-13358.685	6.968	-	-	9.906
L <sub>2</sub>	298.3251322	-10971.26213	2.991	-	-	3.931
CrL <sub>1</sub> L <sub>2</sub>	-----	-----	----	-	-	14.85
NiL <sub>1</sub> L <sub>2</sub>	-----	-----	----	-	-	7.556
CuL <sub>1</sub> L <sub>2</sub>	-----	-----	----	-	-	7.006

**Table (5): Conformation energetic in (in K.J.mol<sup>-1</sup>) and dipole moment (in Debye) for ligands using Gaussian program.**

Ligand	Total energy	$\mu$
L <sub>1</sub>	228.7938415	4.4212
L <sub>2</sub>	299.1957838	2.9937

**Table (6): Comparison of experimental and theoretical vibrational frequencies for primary ligand by HyperChem8 and Gaussian programs.**

Ligand	vC=O	vC=N	vC-S	vN-H	vC=C	vC-H aromatic	
L <sub>1</sub>	Exp.	1705*	1620*	748*	1504*	1504*	3059*
	Hyper.	1902.24 (11.568)	1566.56 (-3.298)	690.35 (-7.707)	1502.68 (-0.087)	1502.68 (-0.087)	3075.10 (0.526)
	Gass.	1951.87 (14.479)	1601.71 (-1.129)	881.73 (17.878)	1535.20 (2.074)	1535.20 (2.074)	3054.19 (-0.157)

**Table (7): Comparison of experimental and theoretical vibrational frequencies for co-ligand by HyperChem8 and Gaussian programs.**

Ligand	v(C=N+C=C)	v(C-H) aromatic	$\delta$ (C-N)	
L <sub>2</sub>	Exp.	1616*	1446*	
	Hyper.	1760.93 (8.968)	3063.20 (2.757)	1395.01 (-3.526)
	Gass.	1697.77 (5.060)	3031.80 (1.704)	1518.71 (5.028)

Where:\* : Experimental frequency

: Theoretical frequency

( ) : Error % due to main different in the experimental measurements and theoretical treatment of vibrational frequency .

**Table (8): Ultra violet spectra of ligands from ZINDO/S calculation and experiment data using HyperChem8 program.**

Ligand	Transition	Experimental	Theoretical (ZINDO/S)
L <sub>1</sub>	n $\rightarrow$ $\pi^*$	29239(342)	343
	n $\rightarrow$ $\pi^*$	32786(305)	303
	$\pi\rightarrow\pi^*$	40485(247)	228
	$\pi\rightarrow\pi^*$	45871(218)	-----
L <sub>2</sub>	n $\rightarrow$ $\pi^*$	30959(323)	-----
	n $\rightarrow$ $\pi^*$	38022(263)	278
	$\pi\rightarrow\pi^*$	43859(228)	218

**Table (9): Comparison of experimental and theoretical electronic transition for ligands from CIS and ZINDO calculation and experiment method using Gaussian program.**

Ligand	Transition	Experimental	Theoretical	
			CIS	ZINDO
L <sub>1</sub>	n $\rightarrow$ $\pi^*$	29239(342)	179.52	303.7
	n $\rightarrow$ $\pi^*$	32786(305)		
	$\pi\rightarrow\pi^*$	40485(247)		
	$\pi\rightarrow\pi^*$	45871(218)		
L <sub>2</sub>	n $\rightarrow$ $\pi^*$	30959(323)	223.64	311.26
	n $\rightarrow$ $\pi^*$	38022(263)		
	$\pi\rightarrow\pi^*$	43859(228)		

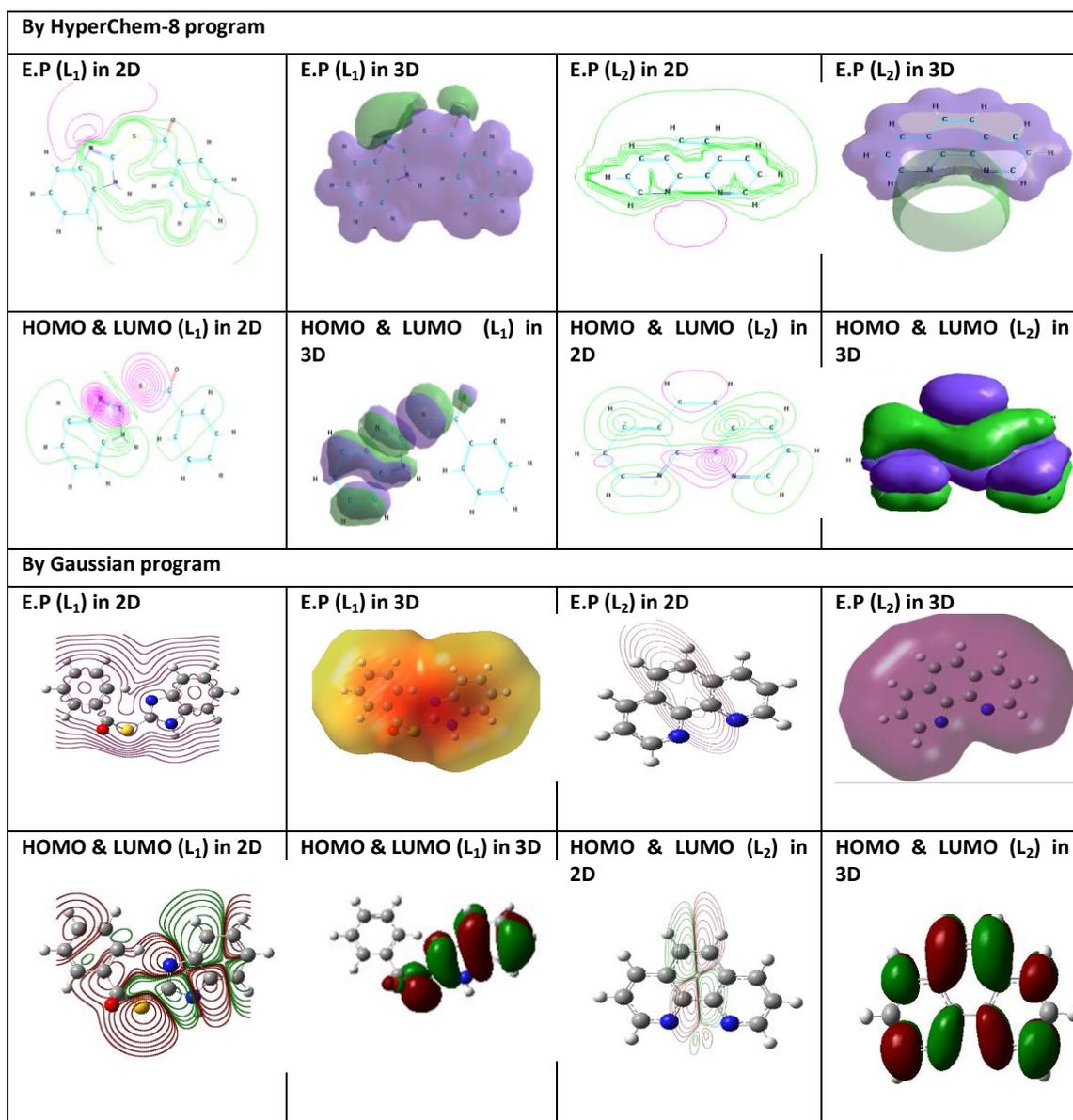


Fig. (2): HOMO,LUMO & electrostatic potential as 2&3D counters for ligands.

### Bactericidal activity of the standard (metronidazole), L<sub>1</sub> and synthesized metal complexes

Antibacterial activity of the prepared ligand and its metal complexes were tested in vitro for antibacterial activity according to the disk diffusion method [22] against the following pathogenic microorganism : *Staphylococcus aureus* (Gram-positive bacteria) and *Pseudomonas aeruginosa* , *E.Coli* and *Salmonella* (Gram-negative bacteria), the prepared agar and petridishes were sterilized by autoclaving for (15 min) at 121°C. the

agar plates were surface inoculated uniformly from the broth culture of the lested microorganisms. In the solidified medium suitable spaced apart holes were made all (6 mm) in diameter compounds (0.01mg of the compounds dissolved in 10ml of ethanol solvent).

These plates were incubated at 37°C for 24hrs, the inhibition zones caused by the various compounds on the bacteria were examined. The results of the preliminary screening test are listed in Figure (3). The data reveal that some complexes have higher activities other have lower than free ligand. These results indicate that the degree of growth

inhibition is highly dependent on (i) the nature of donor atoms (ii) the nature of the metal ion (iii) the chelate effect of the ligand (iv) the total charge on the complex ion (v) the geometrical structure of the complexes (vi) the nature of the counter ions that the neutralize the complex [23]. The chelating theory considerably reduces the polarity of the metal ion mainly

because of partial partnership of positive charge with the donor groups and possible electron delocalization over the whole chelating ligand. Such coordination could also enhance the lipophilic character of the central metal atom, which subsequently favours its permeation through the lipid layer of the cell membranes[24].

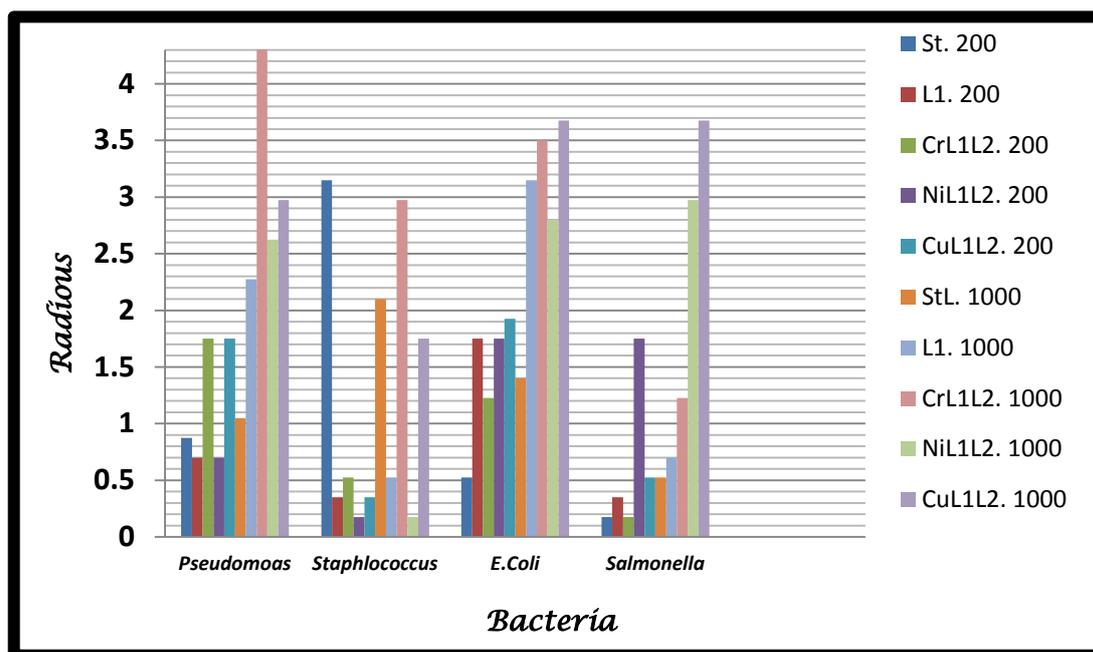


Fig. (3): Antibacterial activities for *standard (metronidazole), L<sub>1</sub>* and their metal complexes

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## معقدات بعض الفلزات الانتقالية مع 2- بنزويل ثايوبنزاميدازول و1-10 فينانثرولين ودراسة فعاليتها المضادة للبكتريا

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### الخلاصة:

تم تحضير الليكاندات الممزوجة ل-2- بنزول ثايوبنزاميدازول ( $L_1$ ) و1-10 فينانثرولين ( $L_2$ ) لايونات العناصر الكروم (III) ، النيكل (II) و النحاس (II). عزلت و شخصت الليكاندات المعقدة المحضرة وبحالتها الصلبة بواسطة تقنيات الأشعة تحت الحمراء والأشعة فوق البنفسجية-المرئية، واطياف الرنين النووي المغناطيسي والامتصاص الذري اللهب، والتحليل الدقيق للعناصر، والحساسية المغناطيسية، ودرجة الانصهار والتوصيلية الكهربائية. الليكاند 2- بنزول ثايوبنزاميدازول يسلك ثنائي السن من خلال ارتباطه بذرة الاوكسجين لمجموعة الكاربونيل وذرة النيتروجين لمجموعة الأيمين. ان الشكل الهندسي المقترح لجميع المعقدات المحضرة ثماني السطوح. اجريت المعالجة النظرية لليكاندات والمعقدات المحضرة في الطور الغازي باستخدام برنامج Gaussian (GaussView (5.0.9) Gaussian Hyper chem.-8، ولليكاندات فقط باستخدام برنامج Gaussian (GaussView (5.0.9) Gaussian). تم تعيين الفعالية المضادة للبكتريا للمعقدات المحضرة ومقارنتها بتلك لليكاند والمادة القياسية المترونيديازول .

الكلمات المفتاحية: الليكاندات الممزوجة، 1،10- فينانثرولين، المعالجة النظرية، الفعالية المضادة للبكتريا.