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Synthesis, Spectral Identification, Antibacterial Evaluationand Theoretical Study of Co, Fe, Rh and Pd Complexes for 2-benzoylthiobenzimidazol

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Abstract:

A new novel series of metalcomplexes are prepared from reactions between 2-benzoylthio-benzimidazole (L) with metal salts of Co (II) , Fe(III) and Rh (III) , while Pd(II) complex was obtained by mixing ligandsof 2-benzoylthiobenzimidazole (L) as primary ligand and bipyridine (L$^{/}$)as secondary ligand as well as palladium chloride as metal salt in an ethanoic medium. The geometry of these compounds were identified using C.H.N.microanalysis, Ultraviolet–visible, Fourier transforms infrared, magnetic susceptibility, molar conductivity and flame atomic absorption (A.A). From the dataobtained by these spectral analyses, the molecular structures for Rh and Fe complexes were proposed to be octahedral geometry. A square planar construction is proposed for Pd(II), while a Tetrahedral Geometry for Cobalt (II)complex. All of the complexes which were prepared displayedobviousconstancy and could be stored for months without showing any considerablealteration. Semi-empirical methods (ZINDO/1, ZINDO/S & PM3) were conducted to assess the heat of formation $\Delta H^{\circ}f$, binding energy ΔEb, and dipole moment for all compounds as theoretic study. The complexes expressnotable biological activities to pathogenic bacteria when inspected on certain bacteria. The synthesized compounds exhibited moderate toverygood antibacterial activity against bacterial strains, i.e., *Escherichiacoli, Staphylococcus aureus & Pseudomonas aeruginosa*.

Keywords:2-Benzoylthiobenzimidazole, Dipole moment, Metal salt, Secondary ligand, Semi-empirical, Pathogenic bacteria.

Introduction:

The interaction of hetrocyclic thiones with metals is still the topic of several as these ligands contain chemistry effective groups and are advantageous model compounds for sulfur containing bases. Heterocyclic 2- thiones bind to a metal in different ways leading to the formation of monomeric polymeric complexes [1] . One of their attractive characters is their acidity, which could affect their chemical reactivity toward transition metal ions and determine the complexes final structure [2]. Azo dyes include the principal group of organic reagent employed in spectrophotometric analysis [3]. They appear in a various industrial application for their color faintness[4]. The coordination chemistry of transition metals resulting from thiol compound attracts the attention of researchers due to different bonding modes exposed by these ligands with both electrons rich and electron poor metals [5]. Schiff base ligands are hypothetically able of creating stable complexes with diverse metal ions [6]. Since, the facile synthesis of Schiff bases many ligands of diverse structure types have been created[7]. Different metal centers requiring diverse coordination modes can be accommodated by the Schiff base, allowing for effective synthesis. [8]. The coordination compounds have the most variety due to the wide range of metal centers and ligand geometries. [9].The aim of the work is synthesis of some metal complexes the type ligand bidentate, studying the pysico – chemical and the suggestion of prepared compounds and study some application of prepared compounds biological activity and theoretical study.

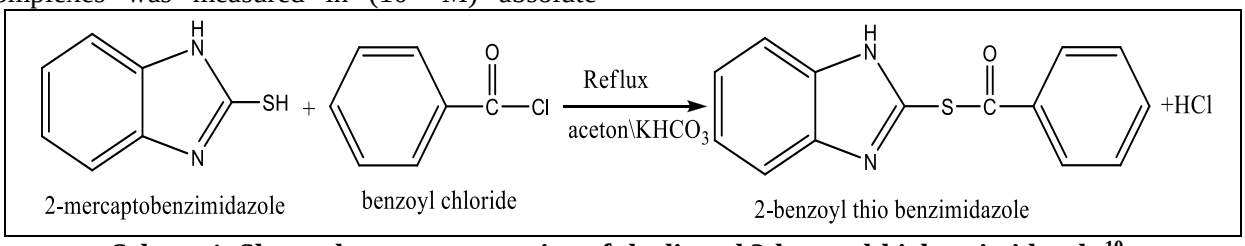
Experimental Part:

Materials and Methods:

All the chemicals used in our work consumed with a high purity and very good quality was exhausted immediately without more decontamination. CsI pellets were used to record FT-IR spectra for all produced compounds on an IR-Prestige-21, Single Beam Path Laser Shimadzu Infrared Spectrophotometer (FT-IR) – 8300.FT-IR spectra for all prepared compounds were recorded using CsI pellets on IR-Prestige-21, Single Beam Path Laser Shimadzu Infrared Spectrophotometer (FT-IR) – 8300. The electronic spectra for the prepared ligands and their metal compounds were measured in DMF using UV-1650 Pc Shimadzu have (1.0 cm) quartz cell at in the range 200-1100 nm. Magnetic properties were used to obtain magnetic moment values. At room temperature, the partition of the Johanson mattey catalytic system is balanced. The molar conductivity for all prepared complexes was measured in (10^{-3} M) absolute ethanol using (WTW) conduct meter. The percentages of the metals in the synthesized compounds were established via Shimadzue Atomic Absorption 680 Flame Spectrophotometer. Microanalysis C.H.N. were done using EM-017.mth instrument.

Preparation of Schiff base (2-benzoylthiobenzimidazole) (L) Ligand

This ligand was synthesized as modified to the literature[10].2-mercapto-benzimidazol (0.06 mole, 9.012 gm) and potassium bicarbonate (0.06 mole, 6.069 gm) dissolved in (120 ml) acetone were combined in a round bottom flask equipped with a magnetic bar stirrer. After 30 minutes of refluxing, benzoyl chloride (0.06 mole) was added drop wise and heated for 4 hours. The color thus formed was cooled in the room temperature and collected by filtration and recrystallized from absolute ethanol and then dried the Table 1 shows the physical characteristics of the produced ligand (1) & the structure in Scheme.1 .



Schema1. Shows the step preparation of the ligand 2-benzoylthiobenzimidazole [10] .

Preparation of new complexes

1- Prepared of Cobalt(II), Iron(III) and Rhodium(III) Complexes:

All the above complexes were preparation a similar way by the usual mixing process between the ligand and metal salts. By addition (1mmole) i.e. (0.22, 0.27 & 0.23 gm) of [($RhCl_3.H_2O$), ($FeCl_3.6H_2O$) & ($CoCl_2.6H_2O$)] and(2 mmole, 0.508 gm) of (2-benzoylthiobenzimidazole)(L) was dissolved in a warm ethanol solution with stirring. The color of the complexes changed in a few minutes. The resulting solution was refluxed for about 2-3 hrs. Then, the precipitated particles were filtered out of the reaction mixture, washed completely with 100% ethanol, and dried recrystallized.

2- **Prepared of Palladium(II)Complex:**

Complex of Pd(II) were prepared by adding equimolar amounts of (2-benzoylethio-benzimidazol) (L) (0.198gm/1mmole) as primary ligand, bipyridine (L/) (0.250 gm/1 mmole) as secondary ligand and (0.17 gm/1mmole) of ($PdCl_2$) as metal salt in ethanoic solution with heat and stirring to reduce the volume of the solution. The result homogeneous solution was reflexed for 2-3 hrs. During this time the product was formed, then filtered off, washed with absolute ethanol and recrystallized. The additional properties for the prepared complex are listed in Table. 1.

3- Biological activity for the ligand and its metal complexes:

Three strains of bacteria (Staphylococcus aureus) as gram positive and (Pseudomonas aeruginosa and E. schriachia coli.) as gram negative were cultivated in nutrient agar media selected to screen the biological activity of the synthesized compounds which dissolved in DMF at concentrations (10^{-3} M) and control with DMF using the disc sensitivity test 11.At 37 °C for 24 hours, the plates were incubated. For more details, check Table 4 for a measurement of the bacterial growth inhibition zone around each compound's disc.

Results and Discussion:

The elemental analysis and atomic absorption show all complexes were preparedin 1:2 (metal: ligand) except Pallidium in 1:1:1 molar ratio. Table 1 summarizes the analytical data as well as certain physical features of the complexes. According to the molar conductance test value, the isolated compounds are crystalline solids,

pigmented, soluble in 100% ethanol, and ionic. The formation and their geometries, stability are further confirmed by Fourier transform FT-IR, UV-Vis spectra, magnetic studies as well as theoretical study.

Table 1. Physical properties, elemental analysis, and atomic spectra of ligands and their compounds

Compounds	Color	Percentage yield	M.P.C°	M.Wt. g.mol⁻	Elemental analysis Found(Calc.)			Metal% Found (Calc.)
					C	H	N	
$C_{14}H_{10}N_2SO$ (L)	Light yellow	86	171-169	254	67.01 (66.14)	4.22 (3.93)	11.53 (11.02)	------
CoL	Greenish blue	72	210 **d**.	673	49.85 (50.23)	3.56 (2.98)	8.30 (8.88)	7.98 (8.75)
FeL	Dark orang	66	156	741	45.26 (45.85)	3.77 (3.93)	7.54 (8.13)	7.00 (7.51)
RhL	Light brown	58	195	733	45.68 (46.00)	2.99 (3.24)	7.61 (7.03)	13.32 (14.00)
PdLL`	Dark brown	72	190	702	54.18 (54.64)	3.12 (3.41)	10.55 (10.62)	8.53 (8.72)

Where **d.** = decompositiondegree.

Infrared Spectra

The free ligand infrared spectrum is compared with infrared spectra of its metal complexes, they provide useful information regarding the coordination behavior of metals and ligands. The carbonyl group (C=O) appears as a peak in the spectrum of 2-benzoylthiobenzimidazol (1705 cm-1). On complexation, this band shifts to a lower frequency, as shown at (1687 cm-1) for Fe^{+3} complex, whereas Pd^{+2}, Rh^{+3}, and Co^{+2} complexes shift to a higher frequency, as seen at (1730, 1722, and 1714 cm-1) for Pd^{+2}, Rh^{+3}, and Co^{+2} complexes, respectively.

The spectrum of free ligand also offer band on (1620 cm^{-1}) have been specified into group azomethine (C=N) For heavy metal complexes Pd+2 and Rh+3, this band changed to a lower wave number and emerged at (1610 & 1606 cm-1). This property is explained by electron transfer from the nitrogen to the metal ion due to coordination[11]. The coordination of electrons from the nitrogen to the metal ion explains this feature. The change to lower frequency could be explained by delocalization of metal electron density into the ligand–system (HOMO-LUMO), where HOMO stands for Highest Occupied Molecular Orbital and LUMO refers for Lowest Unoccupied Molecular Orbital. This band moved to a higher frequency in Fe+3 and Co^{+2} complexes, and was seen at (1635 & 1632).[12] . The shifting of the C=O and C=N peaks on complexation provides useful information about the point of attachment of metal ions to (L) via the carbonyl group's oxygen atom to the metal ion[12] and the iminic nitrogen of the azomethine group[13,14], confirming that 2-benzoylthiobenzimidazol behave as bidentate ligands. The peak at (1351 cm-1) is ascribed to ν(NH) in the free ligand, and the frequency of this band is almost unchanged in spectra for all produced complexes, indicating that the (N-H) group of coordination is not involved.[14].

Metal complexes' infrared spectra indicated a broad band at (3400- 3535 cm^{-1}) region this band was embedded within the ν(OH) of OH group of coordinated water molecules.

Aside from the previously mentioned bands, new bands in the ranges of (547-555 cm-1), (447-474 cm-1), and (312-320 cm-1) have been assigned to temporarily coordinate the nitrogen atom of the azometheine group ν(M-N), the oxygen atom of the carbonyl group (M-O), and the chloride ion with metal ions (M-Cl) [15]. Table. 2 summarizes and characterizes other spectrum bands for ligands and their complexes.

Table 2. Infrared spectrum data of the ligand and its metal complexes(cm^{-1})

Comp.	ν NH	ν C=O	ν C=N	ν C=C	ν C-H arom	γ C-H	δ C-H	ν CSC	ν CS	ν M-N	ν M-O	ν M-Cl	Other bands
$C_{14}H_{10}N_2SO$ (L)	3151	1705	1620	1504	3059	783	1234	1176	748	----	---	---	---
CoL	3159	1714	1632	1499	3059	783	1282	1176	750	555	458	315	3450
FeL	3156	1687	1635	1496	3059	783	1294	1176	756	582	459	312	3330
RhL	3162	1722	1606	1502	3057	785	1290	1174	748	560	447	320	3414
PdLL`	3159	1730	1610 1634	1490	3055	785	1290	1174	750	547	474	317	3400

UV- Visible Spectra Studies

The electronic spectrum of the2-benzoylthiobenzimidazol ligand (L) in DMF solution display four peak is considered a major absorption bands in the ultraviolet visible region. The first and second bands at (342 nm ,29239 cm^{-1})and(305 nm , 32786 cm^{-1}) are due to the (n→π) transition for oxygen atom of C=O group and of –C=N- group, another bands (third and fourth) notice at (247 nm , 40485 cm^{-1}) and (218 nm , 45871 cm^{-1})corresponding to the (π→π*)

The intera-ligand aromatic system shows change(C=C) [16]. The UV-Vis spectrum of dark brown Pd (II) complex showing a peaks at (411 nm, 24300 cm^{-1}), (358 nm , 27932 cm^{-1}) , (259 nm , 33898 cm^{-1}) and (209 nm, 47846 cm^{-1}) were qualified into ($^1A_1g \rightarrow {}^1B_1g$, $^1A_1g \rightarrow Eg$ & L → PdCT) respectively. The value of magnetic susceptibility refers to diamagnetic, thus. the square planer shape was suggested for this new complex agrees with the data of Pd(II)square planner geometry that has been published complexes[16] .

The assignments for the electronic spectra of light brown Rh(III) complex are given in table 3 and it watched bands along with their assignable transition. Low spin has electron is configuration d^6 as t_2g^6 eg^0 the ground term for which in Oh geometry is ^1A_1g. Two bands are expected to appear in visible region and its notice for this prepared complex at (721 nm, 13869 cm^{-1}) and (430 nm, 23255 cm^{-1}) which attributed to ($^1A_1g \rightarrow {}^1T_1g$ and $^1A_1g \rightarrow {}^2T_2g$) and another one band referring to forbidden transition i.e. ($^1A_1g \rightarrow {}^3T_1g$)[17] recorded at (983 nm, 10172 cm^{-1}) in the chart of this complex. The values of ligand filed parameters are estimated and listed in Table. 3.

Fe(III) complex spectrum exhibited three bands appeared at (928 nm ,10775 cm^{-1}) , (560 nm ,17857 cm^{-1}) and (316 nm , 27674 cm^{-1}) assigned to ($^6A_1g \rightarrow {}^4T_1g_{(G)}$, $^6A_1g \rightarrow {}^4T_2g_{(G)}$ and $^6A_1g \rightarrow {}^4A_1g + {}^4Eg_{(G)}$) transitions [18]. For this complex the paramagnets which obtained come in agreement with the reported information for the distorted Oh geometry.

The electronic spectrum of greenish blue of Co(II) complex gave three bands at (650 nm ,15384 cm^{-1}) , (630 nm ,15873) and (607 nm ,16474 cm^{-1}) the average of them transitions which attributed to ($^4A_2 \rightarrow {}^4T_{1(P)}$) transition. The first transition appear at (2.898 nm, 3450 cm^{-1})consequent into the $^4A_2 \rightarrow {}^4T_2$ transition , while ν_2 is estimated calculated by using orgel diagram. All ligand filed parameters are calculated and summarized in Table (3), this complex has paramagnets property. The sites of these bands are appointed with the reported data for tetrahedral system[19].

From the results obtained from the techniques different, the general proposed stereo chemistry structure of complexes can be illustrated as follows in Fig.1

Table 3. Electronic spectra, Molar conductivity and Magnetic moment data of the ligand and its metal complexes

Molecular formula	λmax nm	Absorption Bands(cm^{-1})	Assignments	μ_{eff} B.M.	μs.cm^{-1}	Suggested geometry
	342	29239				
$C_{14}H_{10}N_2SO$	305	32786	$n \rightarrow \pi^*$			
(L)	247	40485	$\pi \rightarrow \pi^*$	-----	-----	-----
	218	45871				
	2.898	3450	$^4A_2 \rightarrow {}^4T_2$			
CoL	1.908	5240 cal.	$^4A_2 \rightarrow {}^4T_1$	3.82	79.0	Tetrahedral
	628	15910	$^4A_2 \rightarrow {}^4T_{1(P)}$			
	928	10775	$^6A_1g \rightarrow {}^4T_1g_{(G)}$			
FeL	650	17857	$^6A_1g \rightarrow {}^4T_2g_{(G)}$	6.12	72.0	distorted
	361	27674	$^6A_1g \rightarrow {}^4A_1g + {}^4Eg_{(G)}$			Octahedral
	983	10172	$^1A_1g \rightarrow {}^3T_1g$			
RhL	721	13896	$^1A_1g \rightarrow {}^1T_1g$	0.00	77.0	distorted
	430	23255	$^1A_1g \rightarrow {}^1T_2g$			Octahedral
	411	24300	$^1A_1g \rightarrow {}^1B_1g$			
PdLL`	358	27932	$^1A_1g \rightarrow Eg$			
	295	33898	L→PdCT	0.00	73.0	Square planner
	209	47846	L→PdCT			

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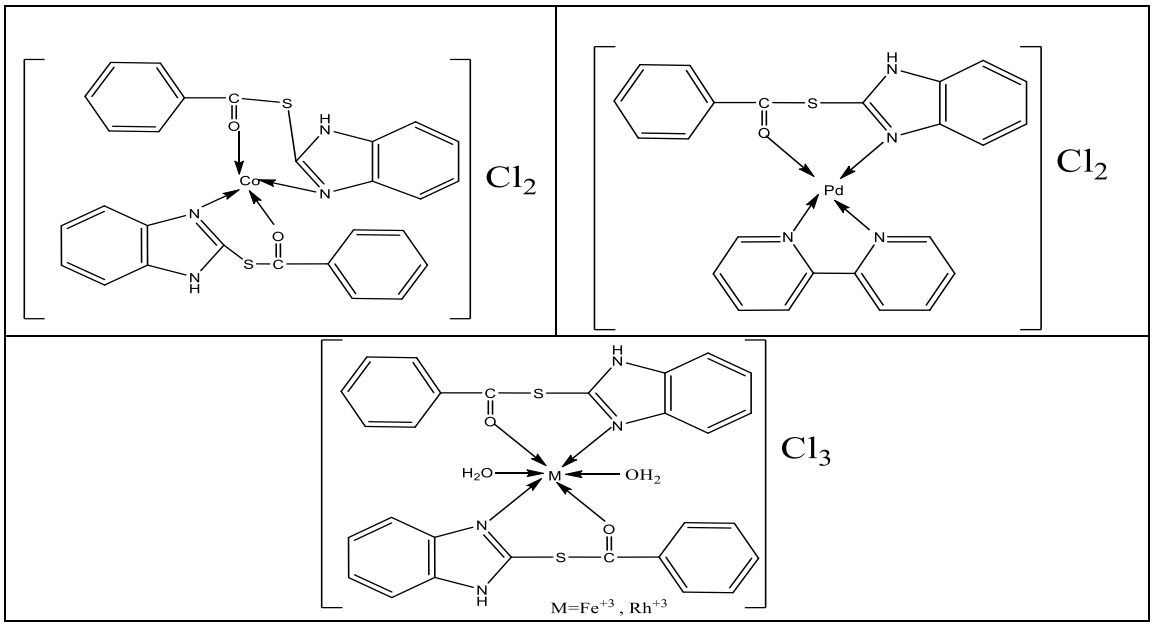


Figure 1. Structure of the proposed synthesis complexes

Antibacterial activity for the prepared compounds:

Antibacterial activity of the prepared ligand and its metal complexes were tested in vitro for antibacterial activity according to the disk diffusion method.

The activity is evaluated against pathogenic bacteria for two of Gram-positive *staphylococcus aureus* and *pseudomonas aerageauosa* and one gram-negative*E-schriochia coli*. The result of antibacterial activities is stated as inhibition zone diameter (mm) as shown in Table 4.Approximately, the results show the impart significant effects of complexes as compared to neat ligand, and this result shows all the new complexes are more toxic as compared with the ligands toward the gram positive microorganism and heavy metal complexes exhibited more toxic as compared with light metal complexes against gram negative bacteria[20].

The nature of the metal ion, the nature of the ligands chelating effect, the nature of donor atoms that coordinate with the metals and the orientation of the ligand around the metal ion, the nature of the metals and their oxidation states, and the geometrical structure of the complexes could all contribute to these results. Metal complexes' higher activity could be owing to metal ions' influence on the normal cell membrane. Metal chelates are excellent for cell penetration because they contain both polar and nonpolar properties. Furthermore, chelation has the capacity to increase or decrease the metabolic potential of bioactive organic molecules. Furthermore, coordination changes lipophilicity, which governs the rate at which molecules enter the cell, allowing the metal complex to become more active than the free ligand. As a result, the metal complexes outperform the uncoordinated ligand in terms of antibacterial activity[21].

Table 4. The antibacterial activity of the ligands and their complexes, as well as the diameter of the inhibition zones (mm).

Comp. Bacteria.	*E. coli (Escherichia coli).*	*Staphlococcus arureus.*	*Pseudomonas aerogenuosa.*
L	+	-	-
L`	+	+	+
DMF	-	-	-
CoL	+	++	++
FeL	+	+++	++
RhL	++	+++	++
PdLL`	+++	++	+++

Where: (-) : No significant Zone,, (+) : Inhibition Zone (4-10),, (++) : Inhibition Zone (10-18)(+++) Zone of Inhibition (18-25).

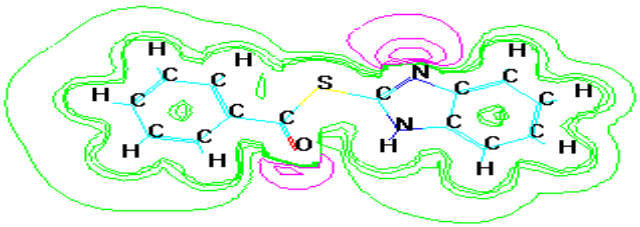
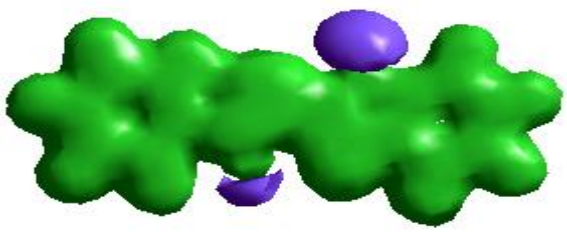
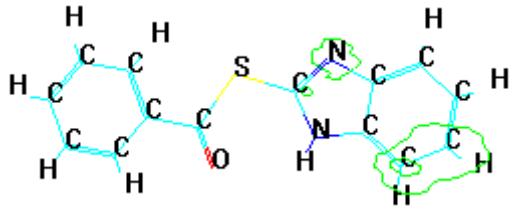
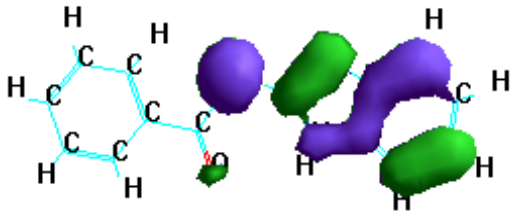
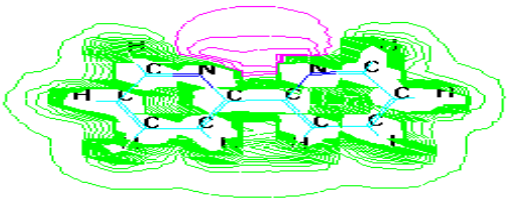
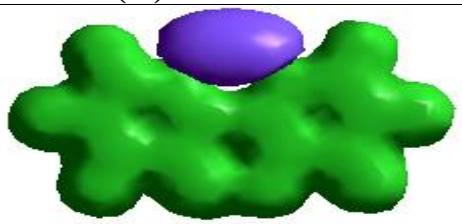
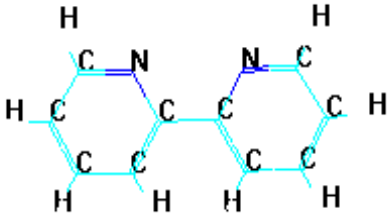
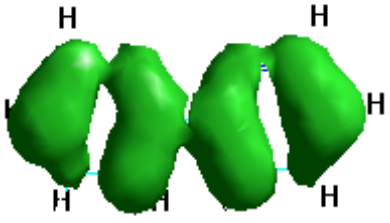
Theoretical Studies:

For the free ligand and its new metal complexes, the heat of formation (ΔH^o_f), binding energy (ΔE_b) and dipole moment (μ) were computed theoretically by Hyperchem-8 using two semi-empirical methods (ZINDO/I & PM3) and

molecular mechanics (AMPER) method [22]. As evidenced by the findings acquired by this software, the complexes are more stable than the ligands directly table 5. Furthermore, the electrostatic potential was computed using the Gaussian program semi-empirical (PM3) technique to investigate the reactive site of the molecules, and the electrostatic potential HOMO and LUMO for free ligand alone was determined fig.2.

Table 5. Using the HyperChem-8 program, conformation energetic (in K.J.mol-1) and dipole moment (in Debye) for ligand (L) and its metal complexes.

Comp.	PM3			ZINDO/1			AMBER
	$\Delta H°_f$	ΔE_b	μ	$\Delta H°_f$	ΔE_b	μ	$\Delta H^{\circ}_f = \Delta E_b$
(L)	60.10323157	-3204.335768	2.554	-6353.732961	-9619.171961	4.145	19.60070734
L`	*64*.3435353	-2287.372465	2.914	-4516.642812	-686.358812	3.862	6.864345919
PdLL`	-101.48430878	-6014.047309	9.062	-12282.59059	-18198.15356	9.511	47.42166464
CoL	---------	--------	----	---------	--------	----	28.84039974
FeL	-108.095908	-6961.595908	6.587	-14333.08172	-21186.58172	6.949	222.1865186
RhL	-278.4125532	-6631.287447	5.16	---------	--------	----	217.9854692

In 2D, E.P (L)	In 3D E.P (L)
	
In 2D HOMO & LUMO (L)	In 3D HOMO & LUMO (L)
	
In 2D E.P(L`)	In 3D E.P (L`)
	
In 2D HOMO & LUMO (L`)	In 3D HOMO & LUMO (L`)
	
In 2D E.P (L)	In 3D E.P (L)

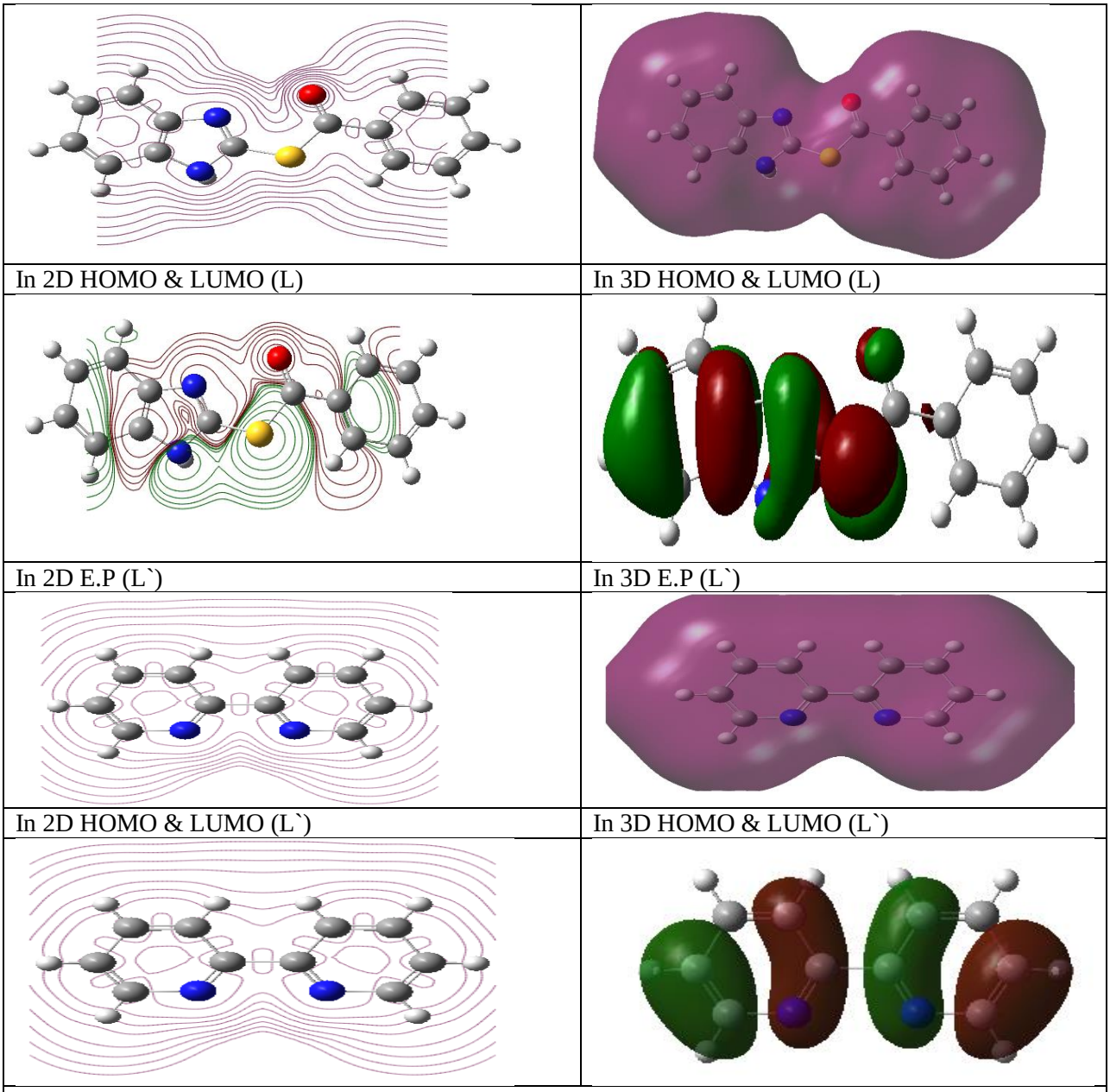


Figure 2. HOMO, LUMO, and Electrostatic Potential as 2D and 3D ligand counters Hyperchem and Gaussian program

Conclusion:

Highly stable to air, moisture and light, metal complexes of 2-benzoylthiobenzimidazol have been successfully prepared simply by reaction the between ligand and metal salts. Also, Pd(II)complex with mixed ligand 2-benzoylthiobenzimidazol & bipyridine have been prepared compounds are characterized by a variety of analytical techniques. The results show that the synthesized ligand have a bidentate nature through O &N atoms with metal complexes and these complexes possess 1 : 2 (M : L) stoichiometry for all metal complexes, except Pd(II) which has 1:1:1 (M:L:L) because it is used as a mixed ligand. The antibacterial properties show all the metal complexes have more biological activity especially heavy metals Rh & Pd compared with the ligands. The theoretical calculation using Hyperchem-8 & Gaussian programs, data gave information about the most stable energy of the structures and reflect that the complexes exhibited to be more stable than the free ligands.

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.

Authors' contributions statement:

The role of first authors I. H. I., has collected and prepared the ligands and the complexes practically , The role of second authors A. S. S.has characterized and analyzed the prepared samples using many techniques, the role of the third authors M. A. has collected the references and written the paper and fourth authors M. F. A. has inspected and reviewed the paper in its find form.

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تحضير، تشخيص طيفي، تقييم الفعالية البايولوجية ودراسة نظرية لبعض معقدات فلزات العناصر الأنتقالية لـ 2- بنزويل ثايوميدازول

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الخلاصة :

تم تحضير سلسلة جديدة لمعقدات بعض الايونات الفلزيه من خلال تفاعل ليكاند 2-بنزويل ثايوبنزامايدزول مع أملاح الفلزات للكوبلت (II)، الحديد (III) والروديو (II)، أما معقد البلاديوم (II) تم تحضيره من خلال مزج 2-بنزويل ثايومايدزولكليكاند أساسي و البابريدينكليكاند ثانوي مع كلورد البلاديوم كملح الفلز في وسط من الأيثانول. تم تشخيص الأشكال لهذه المركبات بواسطة التحليل الدقيق للعناصر، طيف الاشعه فوق البنفسجيه ،تقنية طيف الاشعه تحت الحمراء، الحساسية المغناطيسية، التوصيلية المولارية وتقنية الامتصاص الذري اللهبي. من خلال النتائج التي تم الحصول عليها من التحاليل الطيفية تم اقتراح الشكل الثماني السطوح لمعقدي الحديد والروديوم والشكل المربع المستوي لمعقد البلاديوم ورباعي السطوح لمعقد الكوبلت.اظهرت جميع المعقدات المحضرة استقرارا واضحا ويمكن تخزينها لعدة أشهر دون أي تغيير ملموس . تم أستخدام الطرق شبة التجريبية (ZINDO/S & PM3، ZINDO/ 1) لحساب حرارة التكوين $\Delta H^{\circ}f$ ، وطاقة الاتباطΔEb ، والعزم ثنائي القطب لجميع المركبات كدراسة نظرية . أظهرت المعقدات نشاط بايولوجي ملحوظ تجاة البكتيريا المسببه للامراض عند أخنبارها على انواع مختارة من البكتيريا . أظهرت المركبات المحضرة نشاطاً مضاداً للبكتيريا متوسطاً وجيد جدا ضد السلالات البكتيرية . مثل-*E*-*scherichia coli*، *Staphylococcus* aureusو*Pseudomonas aeruginosa*.

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