Spectroscopic Characterization and Antimicrobial Activities of Some Heavy Metals Complexes of 2-hydroxy phenyl piperonalidene

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Abstract:

An antibacterial and antifungal piperonal-derived compound and its Rh(III), Pd(II), Pt(IV), and Cd(II) metal complexes were synthesized and characterized by spectroscopic methods, conductivity, metal analyses and magnetic moment measurements. The nature of the complexes formed in ethanolic solution was studied following the molar ratio method. From the spectral studies, octahedral geometry was suggested for rhodium (III) and platinum (IV) complexes, while a square planer structure was suggested for palladium (II) complex and a tetrahedral geometry for cadmium (II) complex. Structural geometries of these compounds were also suggested in gas phase by using hyperchem-8 program for the molecular mechanics and semi-empirical calculations. The heat of formation and binding energy for the prepared compounds was calculated by using PM3 and AMBER methods. The theoretically vibration spectra for the imine and its starting material was evaluated by using PM3 method. Preliminary in vitro tests for antibacterial and antifungal activity showed that most of the prepared compounds display a good activity to *(Staphylococcus aureus), (Escherichia coli)* and *(Candida albicans).*

Keywords:- component; Schiff base, piperonaldehyde, heavy metal complexes, Transition metals

Introduction:

Much attention has been devoted by bioinorganic as well as by medicinal chemists to the relationship between the metal ions and their complexes as antitumor [1] and antimicrobial [2] agents. *In vivo* studies have indicated that some biologically active compounds may become more carcinostatic and bacteriostatic upon chelation. Generally, the chelating ligands are polyfunctional molecules which can encage heavy metals in an organic sphere [3]. Schiff base complexes have led to a better understanding of the factors modifying the coordination sphere and the electronic properties of metal ions, and of chelate formation. [3,4]. Furthermore, Schiff bases are used as substrates in the preparation of a number of industrial and biological active compounds [5,6]. Recently, the synthesis and characterization of Schiff base complexes obtained from piperonal were reported [7]. The wide range of applications of the ligand and its complexes were around our interest to prepare a new ligand by the condensation of 2-hydroxy aniline with piperonal. This ligand has both nitrogen and oxygen donor sites. It coordinates with the metal ions as a bidentate manner through enolic moiety and nitrogen atoms of azomethane. The choice of piperonal for the aldehyde moiety in these

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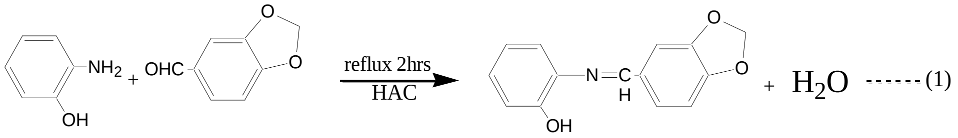
preparations stemmed from the fact that many compounds containing the 3,4-methylenedioxy group have some biological activity [6].

Experimental:

All the chemicals used were of analar of highest grade. Metal salts were used in this study are rhodium trichloride monohydrate $RhCl_3.H_2O$, dichloro bis-benzonitrile $PdCl_2(PhCN)_2$, chloro platinic acid H_2PtCl_6, and cadmium nitrate tetrahydrate $Cd(NO_3)_2.4H_2O$. The metals content of the separated solid chelates were performed using AA-680 Shimadzu Atomic Absorption Spectrophotometer. The electronic spectra of the prepared compounds were recorded on a Shimadzu Uv-160 Spectrophotometer. FTIR spectra of the samples were recorded using FTIR Prestige-21 Spectrophotometer as CsI discs in the wavelength range (4000-200) cm^{-1}. Magnetic susceptibility measurements of the complexes in the solid state were determined using Bruker BM6 instrument at room temperature. The molar conductance of the complexes was measured in DMF as a solvent at room temperature using WTW conductometer type. Melting point apparatus of Gallen Kamp M.F.B-60 was used to measure melting points of the prepared compounds.

Synthesis of 2-hydroxy phenyl piperonalidene (L):

A mixture of (0.15g, 1 mmole) of piperonaldehyde with (0.064 g, 1 mmole) of 2-hydroxy aniline was dissolved in 25 ml of absolute ethanol, three drops of glacial acetic acid were added as a catalyst, the resulting mixture was refluxed on a hot plate with magnetic stirrer for two hours. The precipitate was separated by filtration, washed with diethyl ether and recrystallized from ethanol, then dried under vacuum. The physical properties are shown in (Table 1). The structure of the proposed ligand is shown in (Equation 1).



Synthesis of Metal Complexes:

Imine complexes under investigation were synthesized as follows: The ligand dissolved in 15 ml of absolute ethanol, followed by the addition of 10 ml of metal salt ethanolic solution. The reaction molar ratio was (1:1) for cadmium complex and (1:2) for rhodium, palladium and platinum complexes. The mixture was refluxed for 90 minutes, the coloured products were filtered and washed several times with ethanol then dried under vacuum at 50ºC for two days, the physical properties are shown in (Table 1).

Study of Complex Formation in Solution:

Complexes of imine with metal ions were studied in solution using ethanol as a solvent in order to determine the concentration of metal to the ligand ratio in the complex following molar ratio method [8]. A series of solutions were prepared having a constant concentration 10^{-3} M for each metal ion and ligand. The ratio was determined from the relationship between the absorption of the absorbed light and mole ratio of (M/L). The results of the formed complexes in solution were listed in (Table 1).

Table (1). Physical data of ligand (L) and its metal complexes

Comp.	Colour	m.p. ºC	Yield%	Molar ratio M:L	Metal percentage		Suggested Molecular formula
					found	Calc.	
L	Brown	101-103	88	-	-	-	$C_{14}H_{11}NO_3$
RhL	Brown	195d	84.46	1:2	14.94	14.63	$[RhL_2Cl\ H_2O]$. 3/2EtOH
PdL	Brown	193d	79.65	1:2	20.76	20.96	$[PdL_2]$.2EtOH
PtL	Red-orange	150d	88.75	1:2	24.74	23.86	$[PtL_2Cl_2]Cl_2.H_2O$
CdL	Brown	131d	91.76	1:1	22.88	23.48	$[CdL(H_2O)(ONO)_2]$.EtOH

d = decomposition

Antibacterial and Antifungal Activity:

Disc diffusion method was used for screening the ligand and its complexes [9] for primary selection of the compounds as therapeutic agents. These complexes tested against gram positive *Staphylococcus aureus*, Gram-negative *Escherichia Coli* and pathogenic fungus *Candidia albicans.* Nutrient agar plates were incubated with DMSO of an appropriate dilution of the tested culture and the plates were incubated at the appropriate temperature for 24 hrs.

Results and Discussion:

The newly synthesized Schiff base complexes are stable at room temperature in the solid state. They are generally soluble in DMF and DMSO. The elemental analytical data of the complexes revealed that the compounds have the general formula $[ML_y(H_2O)X]$.nEtOH where M=Rh^{III}, Cd^{II} ; X=Cl^-,ONO_2^- ; n=3/2,1 ; y=2,1 respectively and $[ML_2X_2]Z$ where M= Pd^{II}, Pt^{IV}, X=nil, Cl^- ; Z=2EtOH, $Cl_2.H_2O$ respectively (Figure 1). The analytical data for the ligand and complexes together with some physical properties are summarized in (Table 1) and they are in a good agreement with the proposed stoichiometry of the complexes.

IR spectra (Table 2) provides valuable informations regarding the nature of functional groups attached to the metal atoms. The band at (1627 cm^{-1}) is a characteristic of the azomethane nitrogen atom present in the free ligand and the spectrum showed a weak band at (648 cm^{-1}) assigned to the hydroxyl OH bending vibration [10,11]. This assignment is supported by disappearance of this band when the hydroxyl hydrogen is replaced by the metal except in the spectrum of the Pt(IV) complex. The phenolic C-O stretching asymmetric vibration that appeared at (1265 cm^{-1}) in the ligand [12] underwent a shift toward higher frequencies with splitting in all complexes. This shift indicates the involvement of deprotonated oxygen atom of hydroxyl group in bonding with metal ions [10,11,12] except in the Pt(IV) complex which coordination with protonate oxygen of the ligand. The azomethane band also underwents higher frequencies for the prepared complexes; which is attributed to the complexation through nitrogen of azomethane. This indicates that this ligand behaves as a bidentate through oxygen and nitrogen of Schiff base. The appearance of new bands in the IR spectra of metal complexes as shown in (Table 2) assignable to M-O and M-N in addition to M-X where X= Cl^-, H_2O or ONO_2^- is further indicates the formation of metal complexes, where chlorides and nitrate group compensate the positive charge on the metal ions [11]. A band was observed around

(3417-3155 cm^{-1}) in the spectra of all complexes, assigned to the υ OH suggested the presence of water or ethanol in the crystal lattice of the complexes [10]. No appreciable change is happen in the υ_{asy} (C-O-C) and υ_{sy} (C-O-C) which appeared at 1219 cm^{-1} and 1037 cm^{-1} of the ligand respectively. This mode excluded the participation possibility of oxygen of etheric group to coordinate with metal ions.

Table(2). The most diagnostic FT-IR bands of L and its metal complexes

Comp.	υ C=N	υ C-O	δ -OH	υ C-O-C	υ M-N	υ M-O	Others
L	1627	1265	648	1037 1219	-	-	υ_{OH}=3356
RhL	1678	1284 1265	-	1033 1219	574	463	$\upsilon_{Rh\text{-}Cl}$=408 Coord. δ_{H2O}=864 $\upsilon_{OH\ (H2O,EtOH)}$=3313
PdL	1651	1276 1273	-	1029 1219	582	536	3155 υ_{OH}=
PtL	1666	1273 1270	648	1033 1219	576	480	Pt-Cl=443 $\upsilon_{OH(H2O,OH)}$=3340
CdL	1654	1284 1273	-	1033 1219	543	494	Cd-O =432 ONO_2=1420,1390, 1006 Coord. δ_{H2O}=850 $\upsilon_{OH(H2O,EtOH)}$=3417

Ultraviolet-visible Spectroscopy, Magnetic Moment and Conductivity Measurements:

The electronic absorption spectra of the Schiff base and its complexes in DMF solvent exhibit the important data for the explanation of the transitions occurred. The absorption band of 2-hydroxy phenyl piperonalidene presents at the wavelength (285 nm) may be attributed to ($\pi\rightarrow\pi^*$) transition of the aromatic system. The other band appearing at (350 nm) could be assigned to ($\pi\rightarrow\pi^*$) transition of the imines group[13]. Another absorption band appeared at (435 nm) may be attributed to ($n\rightarrow\pi^*$) transition [14], which is shifted to longer wavelength upon formation of the complexes.

RhL: The electronic spectrum data of the prepared brown complex is presented in (Table 3) along with their assigned transitions. A weak band was observed at (9970) cm^{-1}, which is attributed to the spin-forbidden $^1A_1g\rightarrow{}^3T_1g$ transition [15]. Values of $B^\backslash$, 10 Dq and β were calculated using Tanabe-Sugano diagram for d^6 system. Rhodium(III) complex is a diamagnetic which refers to strong field. Conductivity measurements at 10^{-3} concentration show that the complex is non electrolyte.

PdL: The spectrum of the brown solution of Pd (II) complex showed two bands which are assigned to $^3A_2g\rightarrow{}^3T_2g$ and $^3A_2g\rightarrow{}^3T_1g$ transitions[16,17], (Table 3). A weak band is observed at (13568) cm^{-1}, which is attributed to spin-forbidden $^3A_2g\rightarrow{}^1Eg$ The position of these bands are in a good agreement with that reported for octahedral geometry [17]. The magnetic moment in solid state is found to be zero Bohar Magneton. The conductance measurements indicate the non-conducting behaviour of this complex at 10^{-3} concentration.

PtL: The spectrum of the diamagnetic Pt(IV) complex exhibited two bands in the visible region which were assigned to the transitions $^1A_1g\rightarrow{}^1T_2g$ and L→PtCT. The transition observed at (10020) cm^{-1} is assigned to the spin-forbidden transition $^1A_1g\rightarrow{}^3T_1g$ showing octahedral geometry around Pt(IV) ion [3,18,19]. Conductivity measurements at 10^{-3} concentration showed this complex to be conducting.

CdL: The complex is a diamagnetic as expected for d^{10} ion. The spectrum shows a relative change in the bands position compared to that of the free ligand[18], as listed in (Table 3). At 10^{-3} concentration the conductivity measurements showed to be non-ionic for this complex.

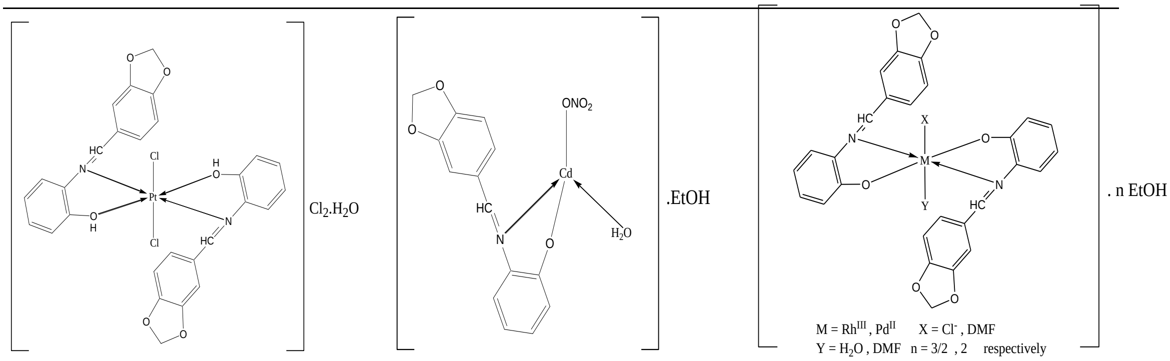


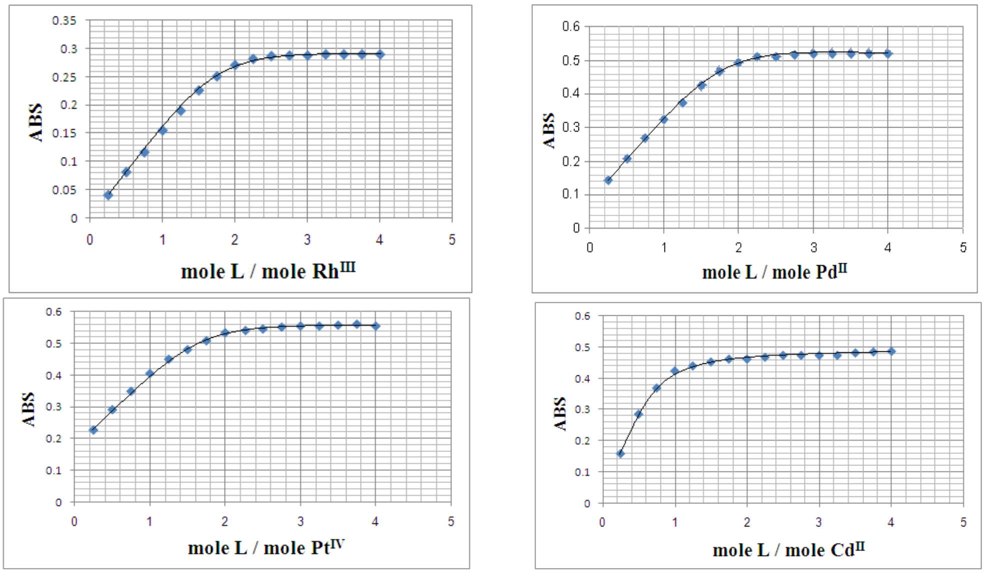
Fig (1). Proposed structure of the prepared complexes

Table (3). Electronic spectra, conductance in DMF solvent and magnetic moment(B.M.) for the present prepared metal complexes of L

Comp.	Absorption Bands (cm^{-1})	Assignments	B	B`	β	Dq/B`	10Dq	15B`	B.M.	μscm^{-1}	suggested geometry
RhL	9970 16393 23529	$^1A_1g \rightarrow ^3T_1g$ $^1A_1g \rightarrow ^1T_1g$ $^1A_1g \rightarrow ^1T_2g$	720	550	0.76	3.3	18150	8250	0.00	45.8	O.h
PdL	13568 20080 26315	$^3A_2g \rightarrow ^1Eg$ $^3A_2g \rightarrow ^3T_2g$ $^3A_2g \rightarrow ^3T_1g$							0.00	47	Oh
PtL	9756 19880 26881	$^1A_1g \rightarrow ^3T_1g$ $^1A_1g \rightarrow ^1T_2g$ L→ PtCT							0.00	91	O.h
CdL	23094 32786 36231	MLCT							0.00	58.2	T.d

Solution Study:

Molar ratio method was followed to determine the M:L ratio. The results of complexes in ethanol solution, suggested that the metal to ligand ratio was (1:1) for cadmium complex (1:2) for the other complexes, which were comparable to those obtained from isolated solid state study, (Table 1) (Figure 2).



Fig(2). Molar ratio plot of the complexes

Theoretical Study:

(i) The program Hyper Chem-8 was used for the semi-empirical and molecular mechanics calculation at optimized geometries energies. The results of PM3 and AMBER methods of calculation in gas phase for heat of formation and binding energy for the ligand and its complexes were calculated and tabulated in (Table 4).

Also PM3 was used for evaluation the vibration spectra of the amine (A) and Schiff base to compare the theoretically calculated wave numbers with experimental values.

Theoretically calculated wave numbers for these ligands showed some deviations from the experimental values. These deviations are generally acceptable in theoretical calculation and are described in (Table 5).

Table (4). Conformation energetic (in kJ.mol^{-1}) for the Schiff base and its metal complexes

Comp.	**PM3**		**AMBER**
	ΔH°_{f}	**ΔE_{b}**	**$\Delta H^{\circ}_{f}=\Delta E_{b}$**
A	-64.52595409	-6603.0587591	-
L	-165.1768378	.5484913793-	-
RhL	.8711631139-	-29323.575490	-
PdL	-1275.103240	-28472.417016	-
PtL	-	-	995.257816
CdL	-286.5516146	-15714.285942	-

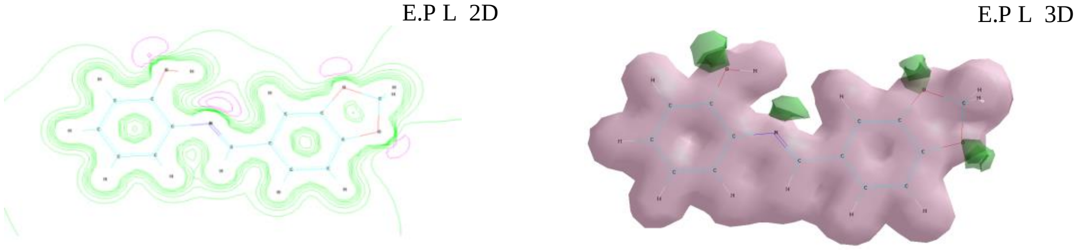
Table (5). Comparison of experimental and theoretical vibrational frequencies for the starting material and Schiff base compound

Symb.	**υ_{asy} NH$_2$**	**υ_{sy}NH$_2$**	**υC-O phenolic**	**υ C=N**	**υOH**	**δOH**	**υ_{as} C-O-C**	**υ_{sy} C-O-C**
A	*3545.84 **3310 ***-7.09	*3487.26 **2990 ***-16.62	*1340 **1275 ***-5.09	_	*3865.04 **3450 ***-12.03	*591.15 **650 ***-9.05	_	_
L	_	_	*1321.23 **1265 ***-4.44	*1836.53 **1627 ***-12.84	*3854.92 **3356 ***-14.86	*553 **648 ***14.62	*1068.37 **1037 ***-3.02	*1215.76 **1219 ***0.265

Where:
* : Theoretical frequency
**: Experimental frequency

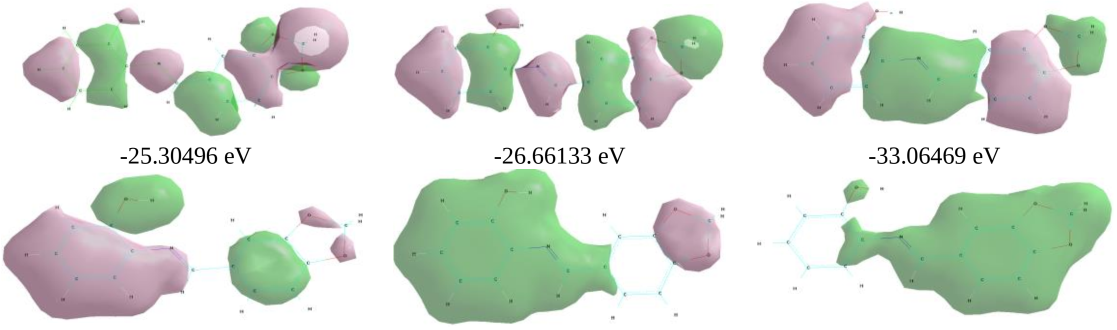
***: Error % due to main difference in the experimental measurements and theoretical treatment of vibrational spectrum.

(ii) Electrostatic potential: It describes the interaction of energy of the molecular system with a positive point charge, so it is useful for finding sites of reaction in molecule positive charge species tend to attack a molecule where the E.P is strongly negative electrophilic attach[20]. The E.P of the free ligand was calculated and plotted as 2D and 3D contour to investigate the reactive sites of the molecules (Figure 3). The results of calculation showed that the LUMO of transition metal ion prefer to react with the HOMO of oxygen and nitrogen atoms of Schiff base ligand (Figure 4).


E.P L 2D

E.P L 3D

Fig(3). Electrostatic Potential as 2D&3D Contours for Schiff bases


-25.30496 eV

-26.66133 eV

-33.06469 eV

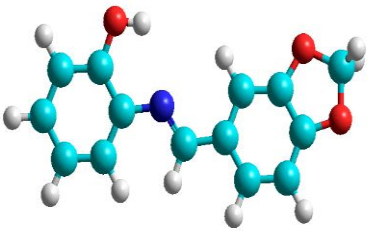
-36.58794 eV

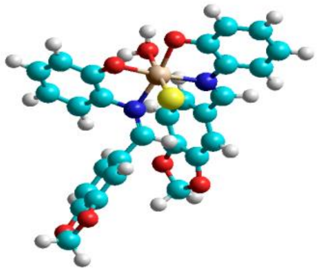
-40.53282 eV

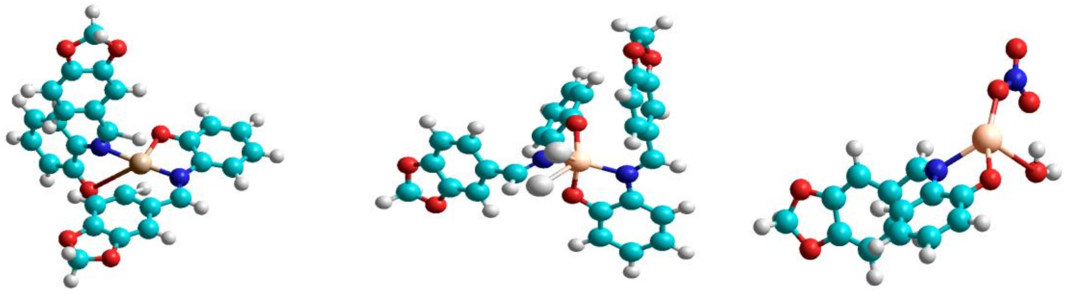
-42.14537 eV

Fig(4). HOMO as 3D Contours for L

(iii) Optimized geometries and energy of metal complexes for the ligand: All theoretically probable structures of metal complexes with ligand have been calculated to search for the most probable model building stable structure. These shapes (Figure 5) show the calculation optima geometries for the imine and its complexes. The results of PM3, methods of calculation in gas phase for the $\Delta H_f°$ and ΔE_b of Rh(III), Pd(II) and Cd(II), while AMBER method used for the Pt(II) complex, and are described in (Table 4).


L


RhL



PdL **PtL** **CdL**

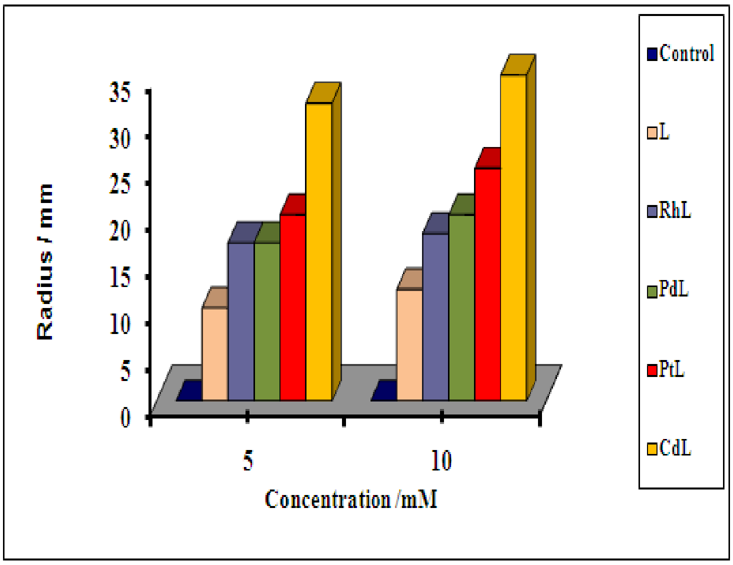
Fig(5). Conformation structure of the ligand and its complexes

Antibacterial and Antifungal Activities:

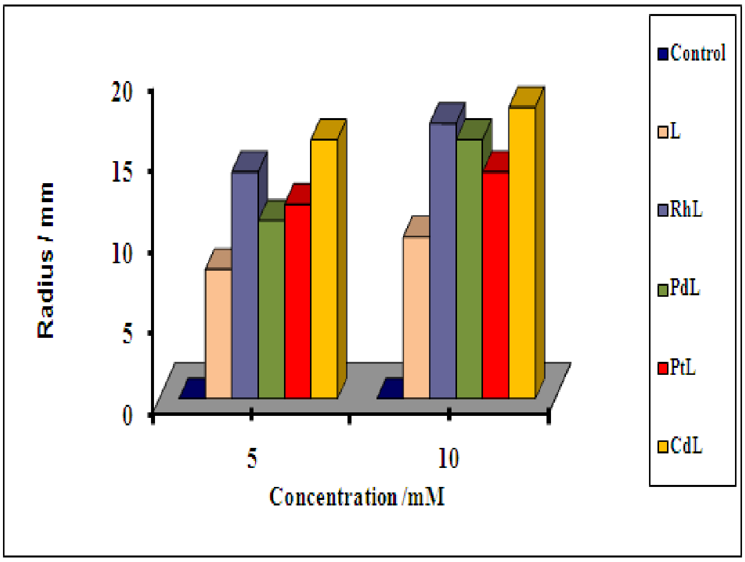
The antimicrobial activities of the prepared ligand and its complexes are given in (Table 6), (Figures 6, 7 and 8). The data reveal that all compounds have good biological activity and some complexes have higher activities than the free ligand. As previously reported, the metal salts do not exhibit antimicrobial activity [21]. Accordingly, the antimicrobial activity of the four complexes can be referred to the increase of their lipophilic character which in turn deactivates enzymes responsible for respiratory processes and probably other cellular enzymes, which play a vital role in various metabolic pathways of the tested bacteria. Also it is proposed that the action of the toxicant is the denaturation of one or more proteins of the cell and this impairs normal cellular process.

Table(6) Diameter of zone of inhibition (mm)

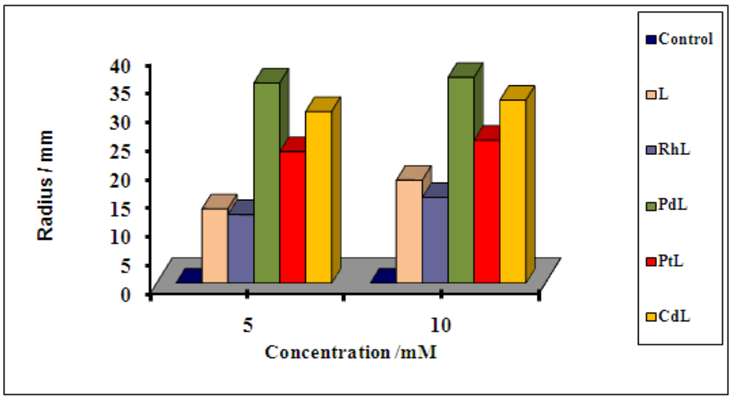
Comp.		**Control**	**L**	**RhL**	**PdL**	**PtL**	**CdL**
Escherichia. Coli	5 mM	-	8	14	11	12	16
	10 mM	-	10	17	16	14	18
Staphylococcus aureus	5 mM	-	10	17	17	20	32
	10 mM	-	12	18	20	25	35
Candida albicans	5 mM	-	13	12	35	23	30
	10 mM	-	18	15	36	25	32



Fig(6). Effect of the ligand and its complexes toward *S.aureus* Bacterial



Fig(7). Effect of the ligand and its complexes toward *E.Coli* bacterial



Fig(8). Effect of the ligand and its complexes toward *C.albican* fungus

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التشخيص الطيفي والفعالية المضادة للميكروبات لبعض معقدات الفلزات الثقيلة لـ 2-هيدروكسي فنيل بيرونالدين

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الخلاصة:

المركب المشتق من البيبرونل كمضاد للبكتريا والفطريات ومعقداته الفلزية Rh(III), Pd(II), Pt(IV) و Cd(II) حضرت وشخصت باستخدام الطرق الطيفية والتوصيلية وتحليل الفلزات وقياسات الحساسية المغناطيسية. تم كذلك دراسة طبيعة المعقد المتكون في محلول الايثانول بأتباع طريقة النسبة المولارية. من الدراسات الطيفية تم اقتراح شكل ثماني السطوح بالنسبة لمعقدات الروديوم (III) والبلاتين (IV) بينما اقترح شكل مربع مستوي بالنسبة لمعقد البلاديوم (II) وشكل رباعي السطوح لمعقد الكادميوم (II). كذلك تم اقتراح الأشكال التركيبية لهذه المركبات نظرياً في الطور الغازي باستخدام برنامج (Hyperchem-8) بتطبيق الميكانيك الجزيئي وشبه التجريبي في الحساب. تم حساب حرارة التكوين وطاقة الترابط للمركبات المحضرة باستخدام طرق PM3 و AMBER. التردد الاهتزازي النظري لمجموعة الايمين ومركبها القياسي قيم باستخدام طريقة PM3. الاختبارات التمهيدية ضد نمو البكتريا و الفطر خارج الجسم اظهر ان معظم المركبات المحضرة ذات فعالية جيدة ضد (*Staphylococcus aureus, Escherichia coli, Candida albicans*).