Synthesis, Spectral Study and Theoretical Treatment of Some Mixing Ligand Complexes of Quinaldic Acid and 1, 10-Phenathroline

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Abstract:

Metal complexes of Cu (II), Fe (III) and Mn (II) with Quinaldic acid (L_1) and 1, 10-Phenathroline (L_2) are synthesized and characterized by standaral physic- chemical procedures (element analysis, metal analysis, FTIR, Uv-Vis, magnetic moment and conductometeric measurements). On the base of these studies, mononuclear and six coordinated octahedral geometry and nonelectrolyte of these complexes have been proposed. The standard heat of formation (ΔH^o_f) and binding energy (ΔE_b) for the free ligands and their complexes are calculated by using the PM3 method at 273K of Hyperchem.-8 program. The complexes are more stable than their ligands. Moreover, the electrostatic potential of free ligands are measured to investigate the reactive site of the molecules, PM3 is used to evaluate the vibrational spectra of the free ligands, the frequencies are obtained approximately agreed with those values experimentally found; in addition, the calculation helps to assign clearly the most diagnostic bands .

Key words: Quinaldic Acid, 1, 10-Phenathroline, Mixing Ligand, Hyperchem.-8 Program, Theoretical Treatment.

Introduction:

Quinaldic acid (QA) and its correspondents offer possible sites for bio-chemically active compounds. They also show wide diversity of medicinal properties that include antitumor [1], antiviral [2], aestrogenic activity [3]. Quinoline carboxylic acid is a strong chelator for many transition metal ions. It also has significant potential applications in the removal and recovery of Al (III) ions from acidic environmental sites of waste, an application that is of chief significance because of the role Al (III) ions play as a neurotoxic contamination and its economic value [4]. Other studies of QA are tested as inhibitors for the corrosion of steel [5], and an established precipitating agent in the gravimetric analysis of metal (II) ions [6]. QA

usually acts as a bidentate chelating ligand in its some metal (II) complexes [7]. Mixed ligand complexes of QA and pyridine derivatives metabolites formed are important signaling agents in neuronal pathways which are vital to the onset of certain diseases [8]. Growths in iron concentrations and picolinic acid have been perceived in Alzheimer [8]. Analogues 2,2-Bipyridine is identified to make stable chelate complexes even with low valent transition metal ions [9]. Today, it is even one of the most widely used chelate systems in coordination chemistry and in recent years has also become a very popular ligand in supramolecular and macromolecular chemistry[10].

Material and Methods:

The chemicals used in this work are all of analytical reagent grade. Furthermore, metal salts used in this study include copper chloride dihydrate $CuCl_2.2H_2O$ from Fluka, manganies chloride tetrahydrate $MnCl_2.4H_2O$ from Fluka, and iron trichloride nano hydrate $FeCl_3.9H_2O$ from BDH. Ligand QH from Merk and 1,10-Phenathroline from RDH. The metal analysis is conducted by a Perkin Elmer 5000 Atomic Absorption Spectrophotometer.

Elemental Analysis (CHN) of compounds is prepared by using EM-034 mth. FTIR spectra are documented on a Shimadzu 8400 Fourier transform spectrophotometer via using CsI disk in the wave number range of 4000-200 cm^{-1},and shimadzu Uv-vis 1600A Ultraviolate spectrophotometer is use to record the electronic spectra by using Quartz cell at a wave length range of 200-1100nm.The molar conductance is calculated in DMF as a solvent at room temperature via coring conductivity Meter 220 with Gallencamp M.F.B-600.01 as a melting point device and magnetic Susceptibility Balance of Johnson matting catalytic system

separation is conducted in room temperature.

Synthesis of Mixed Metal Ligand Complexes:

The method has been used is general to prepare the new complexes by the reaction of a solution containing the co-ligand phen.(5ml) of absolute ethanol, and primary ligand QA (10ml) of the same solvent, are added to a (5ml) warm ethanol of metal salts in molar ratio 1:1:1 . The mixture undergoes heating and reflux operation with stirring for (1.5-3) hrs. The colored precipitates are filtered then washed for several times with ethanol, recrystallized by ethanol-ether mixture. They are dried by using desiccator.

Programs:

HyperChem-8 is a sophisticated molecular modeling environment that is known for its quality, flexibility, and ease of use, uniting 3D visualization and animation with quantum chemical calculations, molecular mechanics, and dynamics. It offers ten semi-empirical methods. Some of them have been developed precisely for the description of organic chemistry too, and commonly good for predicting molecular geometry and energetic. They can be used for prediction vibrational modes and transition structures.

Results and Discussion:
General:

The complexes obtained are colored powders stable for a long time in an open atmosphere. The analytical data for the complexes with some physical properties are summed up in Table (1). All the complexes are cautiously soluble in general organic solvents, the melting points demonstrate that all the complexes decompose prior to melting. Analytical data suggest a ratio of 1:1:1 [M: L_1: L_2] for all metal complexes. Consequently, the format the molar

conductivity corresponding to the Cu(II), Mn (II) and Fe (III) complexes presents low values and in this technique a structural formula of non-electrolyte for these complexes can be assigned. The magnetic moment is consistent with low spin around the iron ion and high spin for both Manganese and Copper ions. Octahedral geometries are recommended for the prepared complexes so that the general formula of these complexes can be shown as: $[ML_1L_2Cl_x(H_2O)_y].ZH_2O$ where $M=Mn^{II}$, Cu^{II}, Fe^{III}; x= 1, 1, 2; y=1, 1, 0; Z=0.5, 1, 2.5 separately.

Infrared Spectra:

The FTIR spectra provide information concerning the nature of the functional group attached to the metal atom. QA may coordinate with metal ions through monodentate, bidentate chelating and bridging according to Nakamato and Deacon& Philips [11]. The infrared spectrum of the solid state of QH indicates that it exists in two toutomeric forms sometime as a neutral molecule (quinolin-2-carboxylic acid) and as a Zwitter ion (quinolinium-2-carboxylate) [12]. The spectrum of the ligand shows a typical broad band in the range (3417-2534) cm^{-1}with the its maximum at 2937 cm^{-1} which refers to the stretching frequency of ν (OH) of carboxylic acid[11]. The absence of absorption of these bands in this region in IR spectra for all complexes confirms the complete deprotonation of ligand in these complexes [13]. Further confirmation comes from the absence of C-O-H bending peak for COOH group at 908 cm^{-1} [14]. The difference of the value (Δν) between the (asy COO$^-$- sym COO$^-$) of all complexes has been compared in order to predict the mode of coordination of metal ions primary ligand HQ as shown in Table (2). The Δν for each complex indicates the monodentate coordination of carboxylic group. The nitrogen atom of ligand also has coordinated with metal ions which is

confirmed in all complexes by shifting the δ bending C=N and appeared in the range (410-390) cm^{-1} [15]. Furthermore, new bands appear by appearance of frequencies in the range (520-542), (416-433) and (320-335) cm^{-1} which is attributed to ν (M-N), (M-O) and (M-Cl) respectively in all complexes. This refers to the ligand which has coordinated as a bidentated with metal ions through oxygen of carboxylic acid and the nitrogen atom [11].Table (2) shows the major bands for phen assigned to the stretching vibrations of ν $_{C=N+ C=C}$ which appears at (1616-1419) cm $^{-1}$ [11, 16, 17]. All bands shift to higher wave numbers in spectra of all complexes compared with spectrum of the free co-ligand. This indicates the coordination to metals through the two Sp^2 hybridized nitrogen atoms [18]. An additional new band appears in the 265, 266 cm^{-1}, this is an additional proof that two nitrogen of co-ligand coordinate with metal ions [16]. A band is observed around (3439-3309) cm^{-1} in the spectra of metal complexes which refers to the presence of water molecules in the crystal lattic or coordinate with metal ions [11].

Electronic Spectra and Magnetic Moment:

Table (3) displays the electronic spectra data of the metal complexes in DMF solvent . The nature of the ligand field around the metal ions has been gathered from the electron spectra.

The electronic spectrum of L_1 shows four main bonds that appear at 45045, 41666,34843 and shoulder band at 30487 cm^{-1} refers to π-π* and 3n-π* transition respectively [19], while L_2 exhibits three bands at 43859, 38022 and 30864 cm^{-1}, due to π→π* and 2n→π* transition [17].

Mn(II) complex: In this study, the brown colour of Mn (II) complex displays two bands at 20408 and 24100 cm^{-1}, spectra assignments are obtained by fitting the observed spectra to

TanabSugao Diagram for d^5 configuration. Table (3) shows the values of ν_1, B`, β and 10Dq computed there form [20].

Two observations have to be pointed out : **(I)** a series of some very weak, and narrow bands have been observed in manganese spectrum. This is expected because only sextet term of the d^5 configuration in Oh stereochemistry is the ^6A_1g, consequently, there can be no spin – allowed transition [20,21].

Furthermore, the energies of the ^4Eg (G) + ^4A_1g (G) terms do not change much relative to the ^6A_1g ground term 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 [20]. **(II)** The value of the nephelauxetic ratio β is evaluated as the ratio of the term separation in the complex. The electronic spectrum coupled with magnetic 4.78BM supports the suggested geometry of this complex [22].

Fe (III) complex: The magnetic measurement shows that iron in its brownish red coloure to be low spin state, which is 2.36 BM, of d^5 configuration. This suggestion is supported by the number of maxima observed in the electronic spectrum of the complex, which shows three maxima at 10869, 15384 and 19841 cm^{-1} may be assigned to the $^2T_2g\rightarrow^4T_1g$, $^2T_2g \rightarrow^4T_2g$ and $^2T_2g\rightarrow^2A_2g + ^2T_1g$ transition[20,23] as shown in Table (3).The ν_1 reach parameter B` and the value of 10Dq are calculated by reference to T. S. D. for $d^5$ configuration. The value of $\frac{55B`}{2}$, which further indicates that the complex is low spin [21,24].

Cu (II) complex: Electronic spectrum of green complex displayed band at 15814 cm^{-1} which is assigned to $^2Eg\rightarrow^2T_2g$ transition, the broadness of the band is due to the ligand field and the Jahn- Teller effect, This absorption prefers the distortion Oh geometry [25]. Moreover, the magnetic moment is 2.1 BM, this value lies within the expected for one electron of mononuclear octahedral [26].

Table (1): Some Analytical and Physical Data for the Ligands and Their Metal Complexes

Compound	Color	M.P °C	Yield %	M.wt g.mol^{-1}	Elemental analysis % Found (calc.)			
					C	H	N	M
$C_{10}H_7NO_2(QH)(L_1)$	White	154-156	--	173.17				
$C_{12}H_8N_2.H_2O$ (L$_2$)	White	100-102	--	198.0				
[MnL$_1$L$_2$ClH$_2$O].1/2H$_2$O	Light Brown	300d	78	487.5	53.52 (54.15)	2.92 (3.89)	7.93 (8.61)	10.58 (11.23)
[FeL$_1$L$_2$Cl$_2$].5/2H$_2$O	Brownish Red	180d	93	542	47.23 (48.708)	2.99 (3.87)	6.54 (7.74)	11.02 (10.33)
[CuL$_1$L$_2$ClH$_2$O].H$_2$O	Green	192d	88	469	55.37 (56.28)	3.96 (4.26)	8.31 (8.95)	12.57 (13.53)

d:decomposition degree

Table (2): Diagnostic FT.IR Bands of the Ligands and Their Metal Complexes (cm^{-1})

Compound	ν asy. COO$^-$	ν sym. COO$^-$	ν C=O	ν C=C +C=N	ν M-N	ν M-O	ν M-N phe	Others
$C_{10}H_7NO_2(QH)(L_1)$	1580	1390	1697	1604, 1534, 1508, 1473	--	--	--	--
$C_{12}H_8N_2.H_2O$ (phe) (L$_2$)	--	--	--	1616, 1589, 1558, 1504, 1446, 1419	--	--	--	ν H2O =3387
[MnL$_1$L$_2$ClH$_2$O].1/2H$_2$O	1597	1394	1695	1622, 1597, 1560, 1516, 1463, 1423	542	416	265	ν H2O =3309 δ H2O=860 MnCl=335
[FeL$_1$L$_2$Cl$_2$].5/2H$_2$O	1591	1385	1695	1625, 1591, 1560, 1504, 1425, 1462	520	433	266	ν H2O =3439 δ H2O=848 FeCl=330
[CuL$_1$L$_2$ClH$_2$O].H$_2$O	1585	1377	1695	1629, 1585, 1568, 1514, 1462, 1421	536	430	265	ν H2O =3342 δ H2O=854 CuCl=321

Table (3): Electronic Spectra Data and Their Assignment of the Prepared New Complexes

Compound	Bands, cm^{-1}	Assignment	B^0 cm^{-1}	Dq/ B	B` cm^{-1}	β	10Dq cm^{-1}	Separation Term
[MnL$_1$L$_2$ClH$_2$O].1/2H$_2$O	11457(cal.) 20408 24100	$^6A_1g \longrightarrow {}^4T_1g$ (G) $^6A^1g \longrightarrow {}^4T_2g$ (G) $^6A_1g \longrightarrow {}^4A_1g+{}^4Eg(G)$	860	1.23CB	745	0.87	9952	11325
[FeL$_1$L$_2$Cl$_2$].5/2H$_2$O	10869 11039 (cal) 15384 19841	$^2T_2g \longrightarrow {}^4T_1g$ $^2T_2g \longrightarrow {}^4T_2g$ $^2T_2g \longrightarrow {}^2A_2g + {}^2T_1g$	1300	3.5 CB	665	0.5	23275	9975
[CuL$_1$L$_2$ClH$_2$O].H$_2$O	15184	$^2Eg \longrightarrow {}^2T_2g$						

Theoretical Study:

(I) The program HyperChem-8 is used for the semi- empirical calculation at optimized geometries energies. The results of PM3 method of calculation in gas phase for heat of formation and ligand and its complexes are calculated and tabulated in (Table 4). Theoretically calculated wave numbers for these ligands show some deviations from the experimental values. These deviations are generally acceptable in theoretical calculation [27] and are described in (Table 5).

Table (4): Conformation Energetic (in KJ.mol^{-1}) for the Ligands and Their Metal Complexes

Compound	PM3	
	ΔH°$_f$	ΔE$_b$
L$_1$	-160.619	-9807.802
L$_2$	297.733	-10971.849
[MnL$_1$L$_2$ClH$_2$O].1/2H$_2$O	-809.750	-22598.260
[FeL$_1$L$_2$Cl$_2$].5/2H$_2$O	-1516.637	-22873.471
[CuL$_1$L$_2$ClH$_2$O].H$_2$O	-465.172	-22308.075

Table (5): A Comparison between Experimental and Theoretical Vibrational Frequencies for the Ligands and Their Metal Complexes (cm-1)

Compound	υ$_{asy}$COO$^-$	υ$_{sym}$COO$^-$	υC=O	υM-N	υM-O	υM-Nphe
L$_1$	*1580 **1516 ***-4.05	*1390 **1245.69 ***-11.58	*1697 **1881.84 ***10.89	---------	---------	----------
L$_2$	-------	-------	-------	---------	---------	---------
[MnL$_1$L$_2$ClH$_2$O].1/2H$_2$O	*1597 **1485.17 ***-7.00	*1394 **1425.98 ***2.29	*1695 **1855.64 ***9.47	*542 **529.47 ***-2.31	*416 **374.07 ***-10.07	*265 **254.76 ***-3.86
[FeL$_1$L$_2$Cl$_2$].5/2H$_2$O	*1591 **1583.56 ***-0.46	*1385 **1428.65 ***3.15	*1695 **1884.47 ***11.17	*520 **529.75 ***1.875	*433 **452.25 ***4.44	*266 **259.44 ***-2.46
[CuL$_1$L$_2$ClH$_2$O].H$_2$O	*1585 **1525.76 ***-3.73	*1377 **1344.40 ***-2.42	*1695 **1863.57 ****9.94	*536 **586 ***9.32	*430 **432.23 **-0.518	*265 **266.87 ***0.705

*Experimental frequencies
**Theoretical frequencies
***Error %

(II) 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 electrophilic attach [20]. 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 (Figure3). The results of calculation illustrate that the LUMO of transition metal ion choose to react with the HOMO of donor atoms in ligands, as shown in Figure (4) via adopting Hyperchem.-8 program.
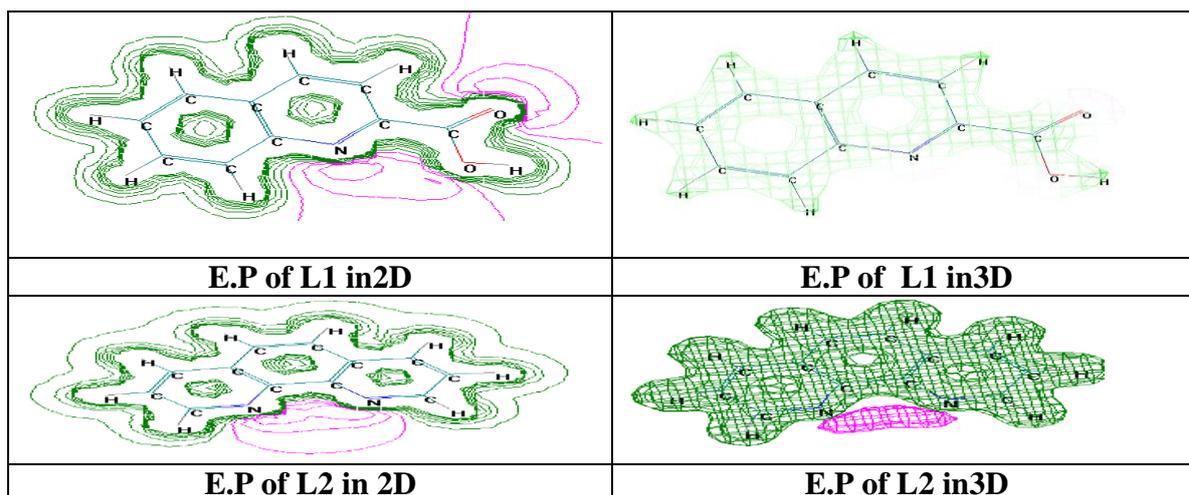
E.P of L1 in2D	**E.P of L1 in3D**
E.P of L2 in 2D	**E.P of L2 in3D**

Fig. (3): Electrostatic Potential as 2D&3D Counters for L1 and L2

HOMO and LUMO in 3D for L1	**HOMO and LUMO in 2D for L1**
HOMO and LUMO in 3D for L2	**HOMO and LUMO in 2D for L2**
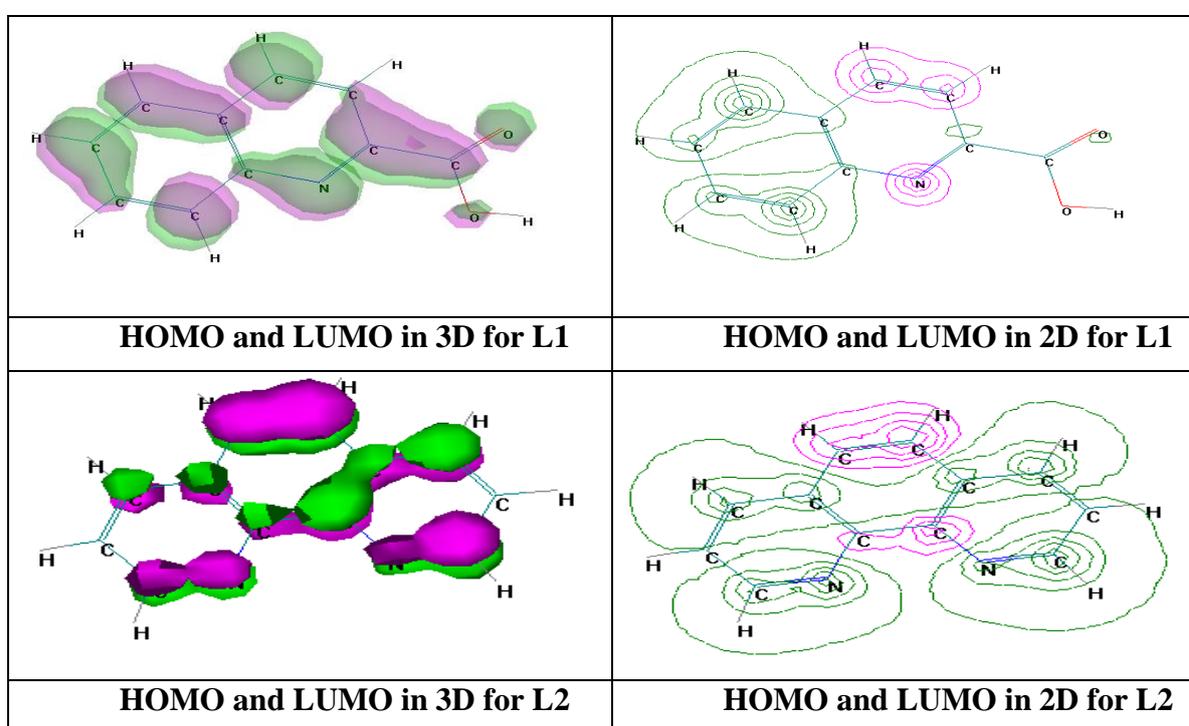
Fig. (4): HOMO and LUMO Sites for the L1 and L2

(III) 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 (5) indicate the calculation optima geometries for the imine and its complexes. The outcomes of PM3 methods of calculation in gas phase for ΔH_f^o and ΔE_b are tabulated in Table (4) for Fe (III), Mn (II) and Cu (II) complexes.

L1

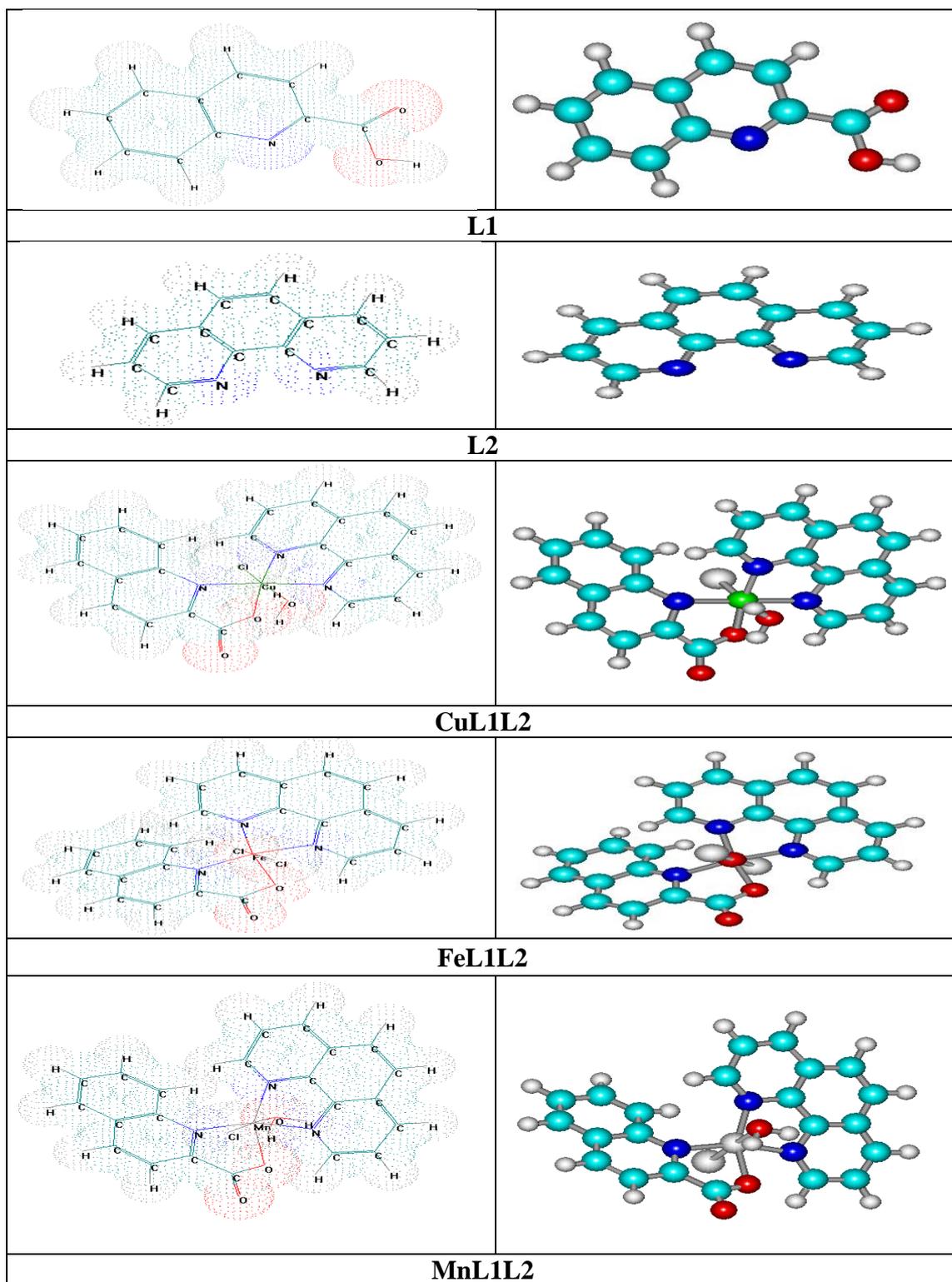**L2**

CuL1L2

FeL1L2

MnL1L2

Fig.(5): Conformation Structure of Ligands and Their Metal Complexes Using Hyperchem.-8. Program
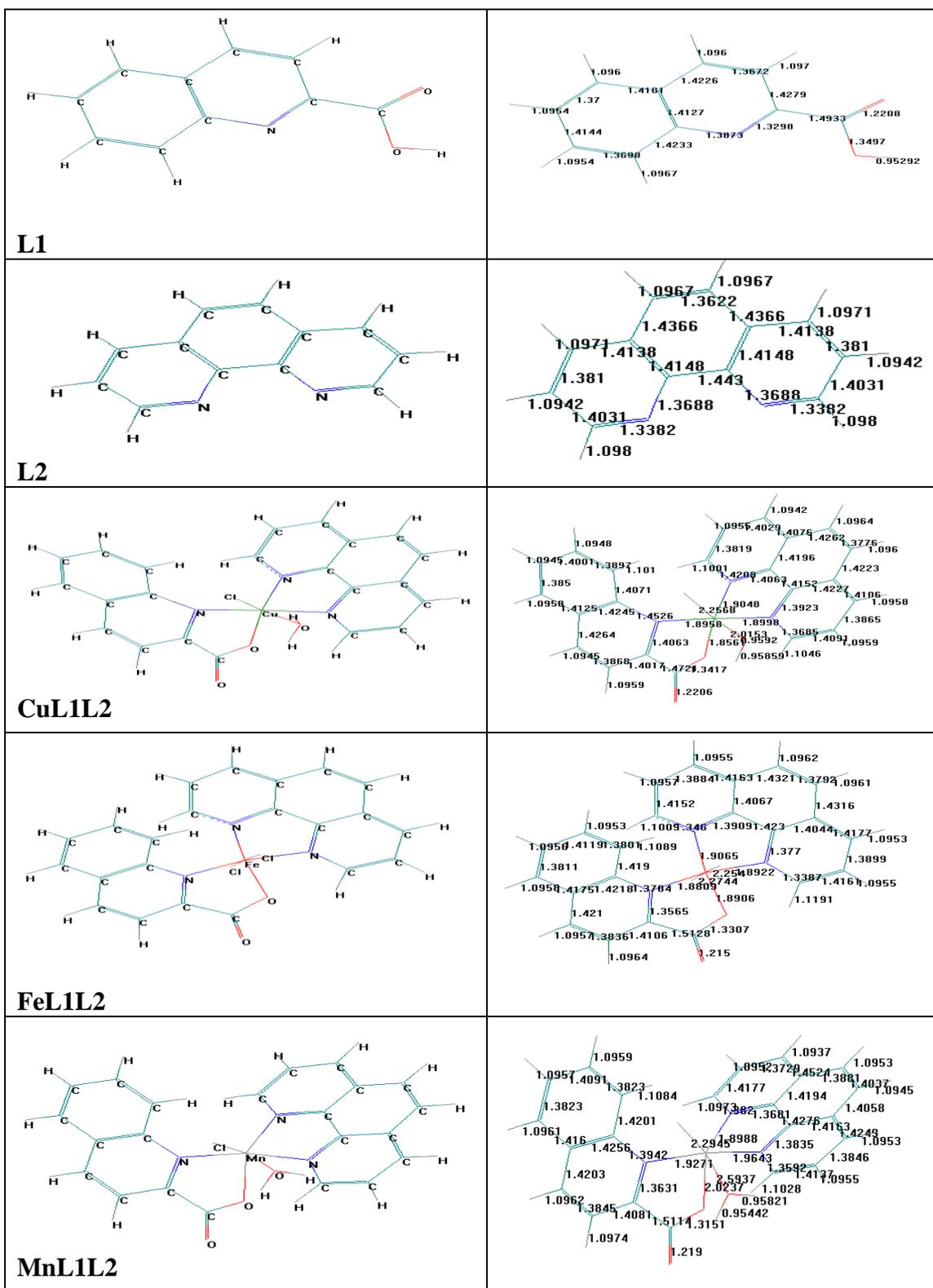
Fig. (6): Bond length of Ligands and Their Metal Complexes Using Hyperchem.-8. Program.

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تحضير و دراسة طيفية ومعالجة نظرية لبعض معقدات مزيج ليكاندات حامض الكوينالديك و 10,1- فينانثرولين

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قسم الكيمياء، كلية العلوم للبنات، جامعة بغداد، بغداد، العراق

الخلاصة:

حضرت معقدات المنغنيز الثنائي والنحاس الثنائي والحديد الثلاثي من مزيج حامض الكوينالديك (L_1) و 10,1- فينانثرولين (L_2) وشخصت بالطرق الفيزيائية والكيميائية (تحليل العناصر ، تحليل الفلزات ، الاشعة تحت الحمراء ، الاشعة المرئية – فوق البنفسجية ، الحساسية المغناطيسية و قياسات التوصيلية الكهربائية) كأساس في هذه الدراسة . اقترح شكل ثماني السطوح سداسية التناسق للمعقدات احادية النواة ، وكانت غير موصلة للكهربائية. تم حساب حرارة التكوين وطاقة التآصر لليكاندات الحرة ومعقداتها بأستخدام طريقة ال PM3 عند درجة 273 كلفن ببرنامج Hyperchem.-8 فوجد ان المعقدات المحضرة اكثر استقراراً من ليكانداتها الحرة، تم تشخيص المواقع الفعالة للجزيئات باستخدام طريقة PM3 لحساب ترددات الاهتزاز لليكاندات الحرة فكانت النتائج متوافقة تقريبا مع القيم العملية بالاضافة الى ذلك ان الحسابات النظرية تساعد في تشخيص معظم الحزم بشكل ادق .

الكلمات المفتاحية: حامض الكوينالديك، 10,1- فينانثرولين، مزيج الليكاندات، برنامج Hyperchem.-8، المعالجة النظرية.