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Synthesis, Spectral Studies, and Theoretical Treatment of some New Metal Complexes with Tridentate Ligand (Schiff and Mannich Base)

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Abstract:

New metal ions complexes of tridentate ligand (1-((dicyclohexylamino) methyl)-3-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrzol-4-ylimino) indolin-2-one) have been synthesized and characterized by chemical-physical analysis. The ligand acts as a tridentate for the complexation reaction with all metal ions. The new complexes, possessing the general formula [M(L)Cl]Cl where M=[Ni(II), Cu(II), Zn(II), Pd(II), Cd(II), Pt(IV) and Hg(II)] ,show tetrahedral geometry. All complexes ,except Pd(II) complex which has a square planar geometry and Pt(IV) which show an octahedral geometry. The geometry of the prepared compounds has been proposed in another method theoretically by using one of the calculation molecular programs (Hyper chem.-6) program. Besides the comparison between the experimental results with the theoretical ones, show that the experimental results are so close to the theoretical counterpart.

Key words: Theoretical studies, Mannich base, Tridentate ligand, Complexes of Dicyclohexylamine

Introduction:

Schiff bases have been playing an important part in the development of coordination chemistry. Schiff bases and their first row transition metal complexes such as Co(II), Ni(II), Cu(II), etc., are reported to exhibit fungicidal, bactericidal, antiviral and antitubarculoral activity [1,2]. They play an important role in both synthetic and structural research because of their preparative accessibility and structural diversity. Isatin (1H-indole-2,3-dione), is a versatile chemical building block, which is able to form a large number of heterocyclic molecules. Isatin itself possesses an extensive range of biological activities [3,4], it is able to participate in a broad range of synthetic reactions, leading to its extensive use as a precursor molecule in medicinal chemistry [5-7] .Recent studies have shown that compounds derived from indolin-2,3-dione are effective against different types of cancer cells. The diketo group can enter into addition and condensation reactions at the C-O bond

[8]. In this paper, we report the synthesis, characterization and theoretical studies of new type ONO tridentate Schiff and Mannich base ligands derived from ,indoline -2,3 –dione,dicyclohexylamine and 4-aminoantipyrine.

Materials and Methods:

Elemental analyses (Carbon, Hydrogen, Nitrogen) are measured by using a Perkin-Elmer CHN 2400 elemental analyzer. The molar conductance of the complexes is determined in DMF at 25±1 °C (10^{-3} M) by using a Jenway 4010 conductivity meter. Magnetic measurements are carried out on a Sherwood Scientific magnetic balance by using the Gouy method. The amount of metal ions is calculated gravimetrically as metal oxides. Electron impact (70 ev) mass spectra are recorded on a Finnegan-MAT model 8430 LC–MS-DS spectrometer. The chloride content is determined by using a potentiometer titration method on a (686-Titro processor -665 Dosimat-metrohmswiss). The uv measurements in solution are carried in a quartz cell by using a Jenway 6405 spectrophotometer, in the range 200–900 nm. FT-IR spectra are recorded in potassium bromide disk on a Bruker FT-IR spectrophotometer in the range 4000-400 cm^{-1}.

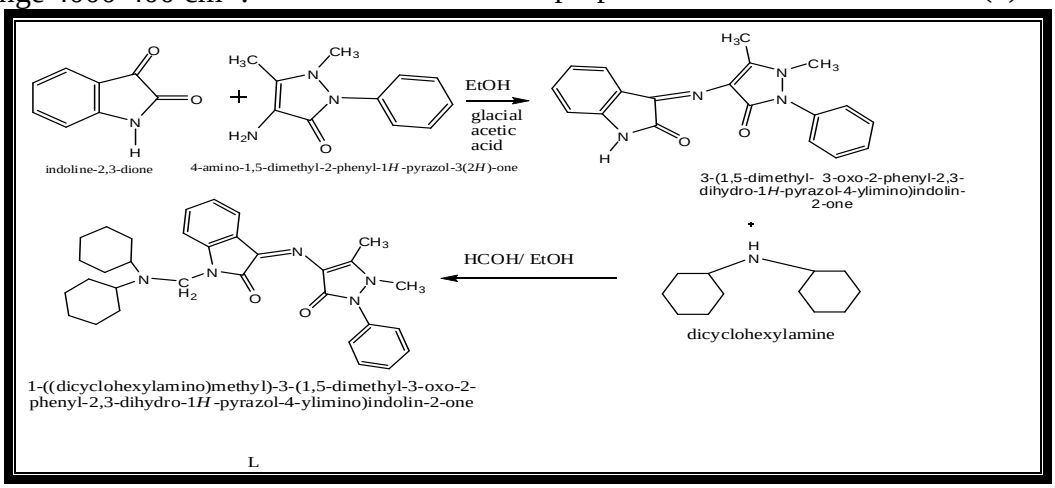
Preparation of Ligand(L) 1-(2,2-dicyclohexylethyl)-3-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-ylimino)indolin-2-one

a- **Preparation of 3-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-ylimino) indolin-2-one(Schiff base).[9]**

(1mol.) indoline -2,3 –dione and (1mol.) 4-amino antipyrine has been dissolved in ethanol and refluxed for (3hrs) by using glacial acetic acid. After standing for approximately (24hrs) overnight, the products are separated by filtration, dried under vacuum and recrystallized from equal percentage of (ethanol: water).

b-1-(2,2-dicyclohexylethyl)-3-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-ylimino) indolin- 2- one (Mannich base) .

A solution of dicyclohexylamine (0.01mol.) in (25ml) of absolute ethanol is added to a solution containing 3-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-ylimino) indolin-2-one and formaldehyde (37% v/v) (0.01 mol each).The reaction mixture is stirred for (24hrs.) and heated at (25-30^{0}C) for (3hrs) then kept under refrigeration for (24hrs.). The products are collected by filtration, dried under vacuum and recrystallized from ethanol as shown in Scheme (1) .The physical and chemical properties are described in Table (1).



scheme (1):Synthesis of 1-((dicyclohexylamino) methyl)-3-(1,5-dimethyl-3-oxo-2-phenyl 1,-2,3-dihydro-1H-pyrzol-4-ylimino)indolin-2-one (L)

Preparation of Complexes:

The preparation of all complexes is essentially the same and so a generic description will be presented. To a solution of (L) (1mmole) in ethanol, is slowly added a solution of metal salt ($NiCl_2.6H_2O$, $CuCl_2.2H_2O$, $PdCl_2$, $ZnCl_2$, $CdCl_2$, $H_2PtCl_2.6H_2O$ and $HgCl_2$) in ethanol – water solution (1:1 v\v) with stirring. The mixture is refluxed for (3-6hrs). The colored precipitated solid is filtered, washed several times with ethanol and dried under vacuum, Scheme (2) some physical properties are listed on Table (1).

Computational Chemistry

Computational chemistry is one of the chemical applications to solve chemical problems using mathematical applications based on molecular shape (sample molecular) .To build a molecular model accurately based on the electronic build method that relies on quantum mechanics , you must increase the storage capacity and increase the processor speed ,so was the introduced another method (semi-empirical method) to resolve this problem by introducing experimental spectral values for the purpose of speeding up the calculation calendar style treatment[10].

Results and Discussion:

The elemental analysis shows 1:1 (metal:ligand) stoichiometry for the complexes .The analytical data together with some physical properties of the complexes are summarized in Table (1).They agree well with the formula[M(L)Cl]Cl, where [M= Ni(II), Cu(II), Zn(II), Cd(II) ,Pd(II) and Hg(II)], $[Pt(L)Cl_3]Cl$,L= 1-((dicyclohexylamino) methyl) -3- (1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H- pyrazol- 4-ylimino) indolin-2-one. The complexes are air-stable solids, soluble in some solvent such as DMF and DMSO, partly soluble in CH_3OH, $CHCl_3$, CH_2Cl_2 and insoluble in other common organic solvents. The molar conductance values of the complexes indicate their 1:1 electrolytic nature.

Table (1) Analytical and Physical Data of the Ligand and its Complexes

Compounds	Color	M. P. °C	Yield %	Elemental analysis, (found) Calc.%					Suggested Formula M. wt (g mol^{-1})
				C	H	N	M	Cl	
L	Orange Reddish	156-158	87	73.11 (74.16)	7.48 (7.17)	13.32 (12.40)	-	-	$C_{32}H_{39}N_5O_2$ 525.31
NiL	Yellow greenish	240d	70	58.65 (60.02)	6.00 (5.83)	10.69 (10.04)	8.96 (9.23)	10.82 (10.98)	$C_{32}H_{39}N_5O_2Cl_2Ni$ 655.28
CuL	Brown	240d	75	58.22 (59.02)	5.95 (5.59)	10.61 (10.04)	9.63 (10.00)	10.74 (9.98)	$C_{32}H_{39}N_5O_2Cl_2Cu$ 660.14
ZnL	Light Orange	249d	68	58.06 (59.00)	5.94 (5.59)	10.58 (10.14)	9.88 (10.02)	10.71 (9.98)	$C_{32}H_{39}N_5O_2Cl_2Zn$ 662.00
CdL	Light Orange	265d	75	54.21 (53.34)	5.54 (5.59)	9.88 (9.14)	15.85 (16.80)	10.00 (9.98)	$C_{32}H_{39}N_5O_2Cl_2Cd$ 709.00
HgL	Light Orange	287d	75	48.21 (48.82)	5.93 (5.59)	8.79 (8.14)	25.16 (24.99)	8.89 (7.98)	$C_{32}H_{39}N_5O_2Cl_2Hg$ 797.18
PdL	Brown Reddish	245d	75	54.67 (54.82)	5.59 (5.59)	9.96 (9.14)	15.14 (14.54)	10.09 (8.98)	$C_{32}H_{39}N_5O_2Cl_2Pd$ 703.01
PtL	Brown Reddish	230d	79	44.56 (45.02)	4.56 (5.03)	8.12 (8.14)	22.62 (22.00)	16.44 (16.98)	$C_{32}H_{39}N_5O_2Cl_4Pt$ 862.57

d=decomposition degree

IR Spectra

The IR data of the spectra of ligand and their complexes are presented in Table 2. The IR spectrum of the compound (L) shows characteristic bands at 3151-3089, 2966-2897, 1724-1651 and 1620 cm^{-1} due to the ν(CH) aromatic, ν(CH) aliphatic, ν(C=O), and ν(C=N) functional groups respectively for the ligand [11] . The IR spectra of the complexes exhibit shift of ν (C=O), and ν (C=N) bands to lower frequencies [(24-16) and (21-8) cm^{-1}] bands of the ligand is observed at 1620 cm^{-1} and this band is shifted to the lower frequencies [12-14]. This indicates the involvement of the ligand with the metal ions through the O, O carbonyl groups and N azomethine group atoms [15]. The spectra of all the complexes show additional medium intensity bands in the range (590-510) and (486-412) cm^{-1} assigned to the υ(M-N) and υ(M-O), respectively[14, 15].

Table (2) FTIR Spectral Data for the Ligand and its Metal Complexes (cm^{-1})

Compound	υC-H ar.	υC-H alip.	υC=O	υC=N	υM-N	υM-O
L	3151 3089	2966 2897	1724 1651	1620	-	-
NiL	3097 3019	2950 2887	1707 1637	1588	568 510	430
CuL	3110 3009	2940 2912	1708 1632	1604	590 557	460 444
ZnL	3117 3006	2937 2921	1705 1630	1576	577	439 420
CdL	3120 3060	2935	1701 1640	1581	580 545	470 417
HgL	3118	2959 2939	1700 1624	1578	590 530	412
PdL	3120 3035	2944	1704 1639	1591	590 572	485
PtL	3098 3042	2938 2841	1701 1643	1600	516	486

ar= aromtic, ali=aliphatic

Electronic Spectra, Magnetic Moment and Conductivity Measurements:

The spectral data of the ligand and its complexes in DMSO are described on Table (3). The ligand exhibits strong absorption bands at (282,330) and 348 nm attributed to π→ π* and n → π*, respectively [16,17], which is shifted to longer wavelength upon formation of the complexes.

NiL: The spectrum of yellow greenish of Nickel(II) complex shows a band at 13774 cm^{-1} region due to $^3T_{1(F)} \rightarrow {}^3T_{2(F)}$ υ_1. This result is in good agreement with the expected tetrahedral geometry for this complex since the other band at (23696, 25974) which refers to $^3T_{1\,(F)} \rightarrow {}^3A_{2\,(F)}\upsilon_2$ and $^3T_{1(F)} \rightarrow {}^3T_{1(P)}\ \upsilon_3$ located is usually below the instrumental limit [18] .The magnetic moment value (3.6) BM for the complex confirmed the presence of two unpaired electrons and tetrahedral environment [19-20]. The increase in the magnetic moment is expected due to presence of contribution spin orbital coupling.

CuL:The electronic spectrum of Cupper(II) complex shows a broad band at 16474 cm^{-1} which may be assigned due to the combination of transition $^2T_2 \rightarrow {}^2E$ in tetrahedral field .Another high intensity band at 24096 and 25000cm^{-1} is due to charge transfer transition [21-22]. The magnetic moment value of this complex is 1.8BM [19-20].

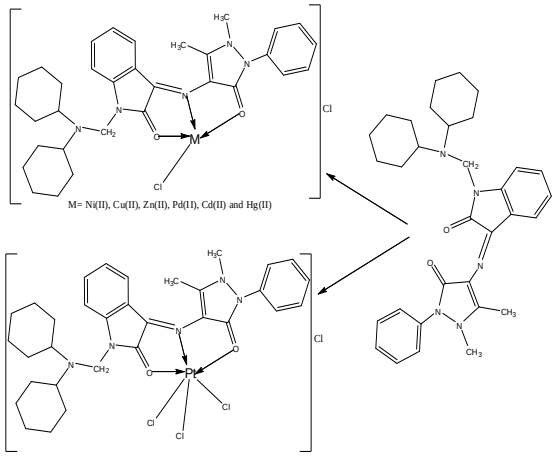
ZnL, CdL, HgL: Due to their diamagnetic properties and no d-d

transition the spectra of these complexes exhibit only a strong charge transfer band around 30769 cm^{-1}, 31250 cm^{-1} and 31250 cm^{-1} for Zn (II), Cd(II) and Hg(II) respectively .Based on analytical data, the suggested tetra coordinate complexes may acquire tetrahedral geometry [23-24].

PdL: The spectrum of the brown reddish of Palladium (II) complex show three bands which are assigned to C.T, $^1A1g \rightarrow {}^1B_1g$ and $^1A_1g \rightarrow {}^1A_2g$ transitions (Table 3). The positions of these bands are in good agreement with that reported for square planner geometry [25]. The magnetic moment in solid state is found to be zero Bohar Magneton [19,20].

PtL: The spectrum of the diamagnetic Platinum (IV) complex exhibits three bands in the visible region which are assigned to the transitions ($\pi \rightarrow \pi^*$), $^1A_1g \rightarrow {}^1T_2g$ and $^1A_1g \rightarrow {}^1T_1g$. The transition observed is attributed to octahedral geometry around Pt(IV) ion [25-27].

The conductance measurements indicate the conducting behavior for all complexes at $(1x10^{-3})M$.



Scheme (2): Suggested Structure for the Prepared Complexes

Table (3) Electronic Data and Molar Conductivity for the Metal Complexes

Complexes	*Molar Conductive $cm^2 s\ mole^{-1}$in DMSO*	*μ_{eff} B.M Found (calculate)*	*λ_{max} nm*	*$\acute{v}cm^{-1}$*	*ε_{max} $Lmol^{-1}cm^{-1}$*	*Assignment*	*suggested geometry*
NiL	73	3.6 (2.82)	385 422 626	25974 23696 13774	1097 16 11	$^3T_{1(F)} \rightarrow {}^3A_{2(F)}$ $^3T_{1(F)} \rightarrow {}^3A_{2(F)}$ $^3T_{1(F)} \rightarrow {}^3A_{2(F)}$	T.d
CuL	69	1.8 (1.73)	400 415 607	25000 24096 16474	564 563 31	C. T C. T $^2T_2 \rightarrow {}^2E$	T.d
ZnL	71	Diamagnetic	325	30769	113	ILCT	T.d
CdL	66	Diamagnetic	320	31250	324	ILCT	T.d
HgL	69	Diamagnetic	320	31250	324	ILCT	T.d
PdL	67	Diamagnetic	518 598 899	19305 16722 11123	5100 800 300	C.T $^1A_1g \rightarrow {}^1B_1g$ $^1A_1g \rightarrow {}^1A_2g$	S.P
PtL	75	Diamagnetic	589 587 892	25706 16528 11428	640 100 80	$\pi \rightarrow \pi^*$ $^1A_1g \rightarrow {}^1T_2g$ $^1A_1g \rightarrow {}^1T_1g$	O.h

Mass Spectrum

The electron impact spectrum of ligand (L) confirms the probable formula by showing a peak at (525.4 m/ z) cores bonding to Mannich Schiff base moiety [($C_{32}H_{39}N_5O_2$) calculated by an atomic mass 525.4]. The series of peaks at m/z 205, 204, 194, 75 and 36 are attributed to the molecular ion fragments: ($C_{11}H_{15}N_3O$), ($C_{11}H_{14}N_3O$), ($C_{13}H_{24}N$), (C_3H_9NO) and (H_6NO) respectively. The fragmentation pattern for copper complex confirms the probable formula by showing a peak at (660M /Z) cores bonding to Cu complex moiety ($C_{32}H_{39}N_5O_2CuCl_2$).by calculating the atomic mass 660] , the series of peaks at

m/z 620 ,430 ,429, 205 ,and 204 are attributed to the fragment molecular ions ($C_{32}H_{35}$ ClN_5O_2Cu), ($C_{26}H_{31}N_5O$), ($C_{26}H_{30}N_5O$), ($C_{11}H_{15}N_3O$) and ($C_{11}H_{14}N_3O$) respectively. The fragmentation pattern for zinc complex confirms the probable formula by showing a peak at (662M /Z) cores bonding to Zn complex moiety ($C_{32}H_{39}$ $Cl_2N_5O_2Zn$) by calculating the atomic mass 662], the series of peaks at m/z 620, 205 and 204 are attributed to the fragments of molecular ions ($C_{32}H_{33}ClN_5O_2Zn$), ($C_{11}H_{15}N_3O$) and ($C_{11}H_{14}N_3O$) respectively .

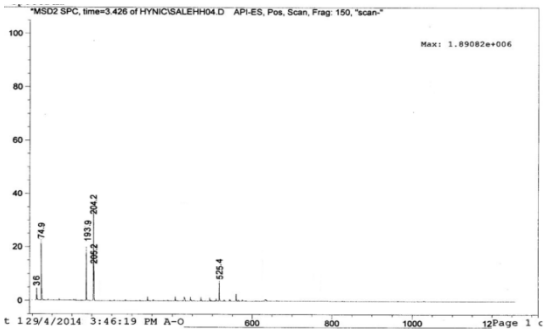


Fig.(1) LC-Mass of Ligand

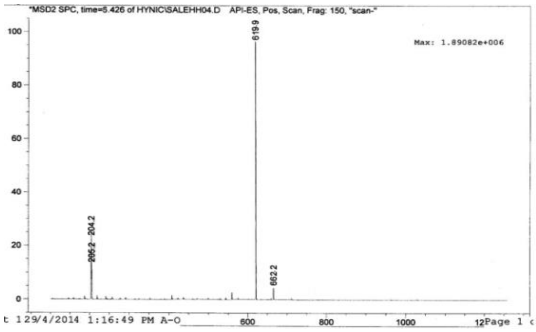


Fig.(2) LC-Mass of Zn L

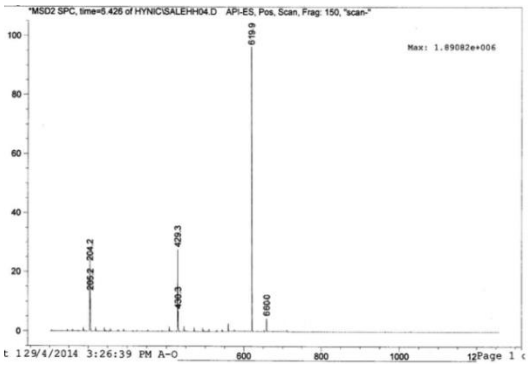


Fig.(3) LC-Mass of Cu L

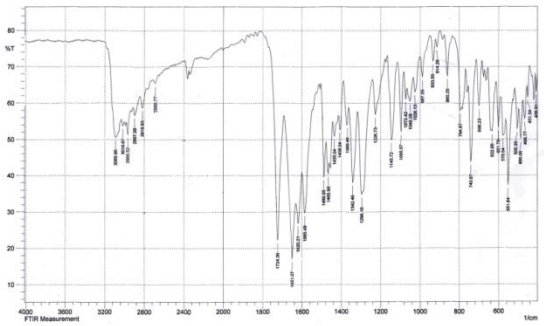


Fig.(4) Spectrum of Ligand

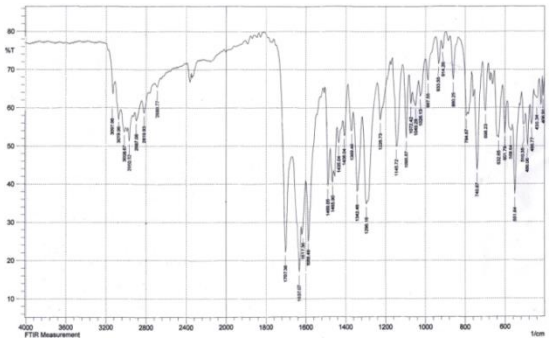


Fig.(5) Spectrum of NiL Complex

Theoretical Energies and Dipole Moment

The program Hyperchem-6 is used for the semi-empirical and molecular mechanic methods to calculate the heat of formation ($\Delta H°f$), binding energy (ΔEb) and dipole moment (μ) for ligand and their prepared complexes by different method PM3, ZINDO/1 and AMBER methods, in addition to calculating some identification vibration in IR spectra and molecular orbital HOMO and LUMO for ligand. Fig. (7,8) and Table (4) show a comparison of experimental and theoretical vibrational frequencies for Ligand and NiL complex**,** while Table (5) shows values heat of formation ($\Delta H°f$), binding energy (ΔEb) and dipole moment (μ) for 1-((dicyclohexylamino) methyl)-3-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrzol-4-ylimino) indolin-2-one and all prepared complexes, results show stability of all complexes.

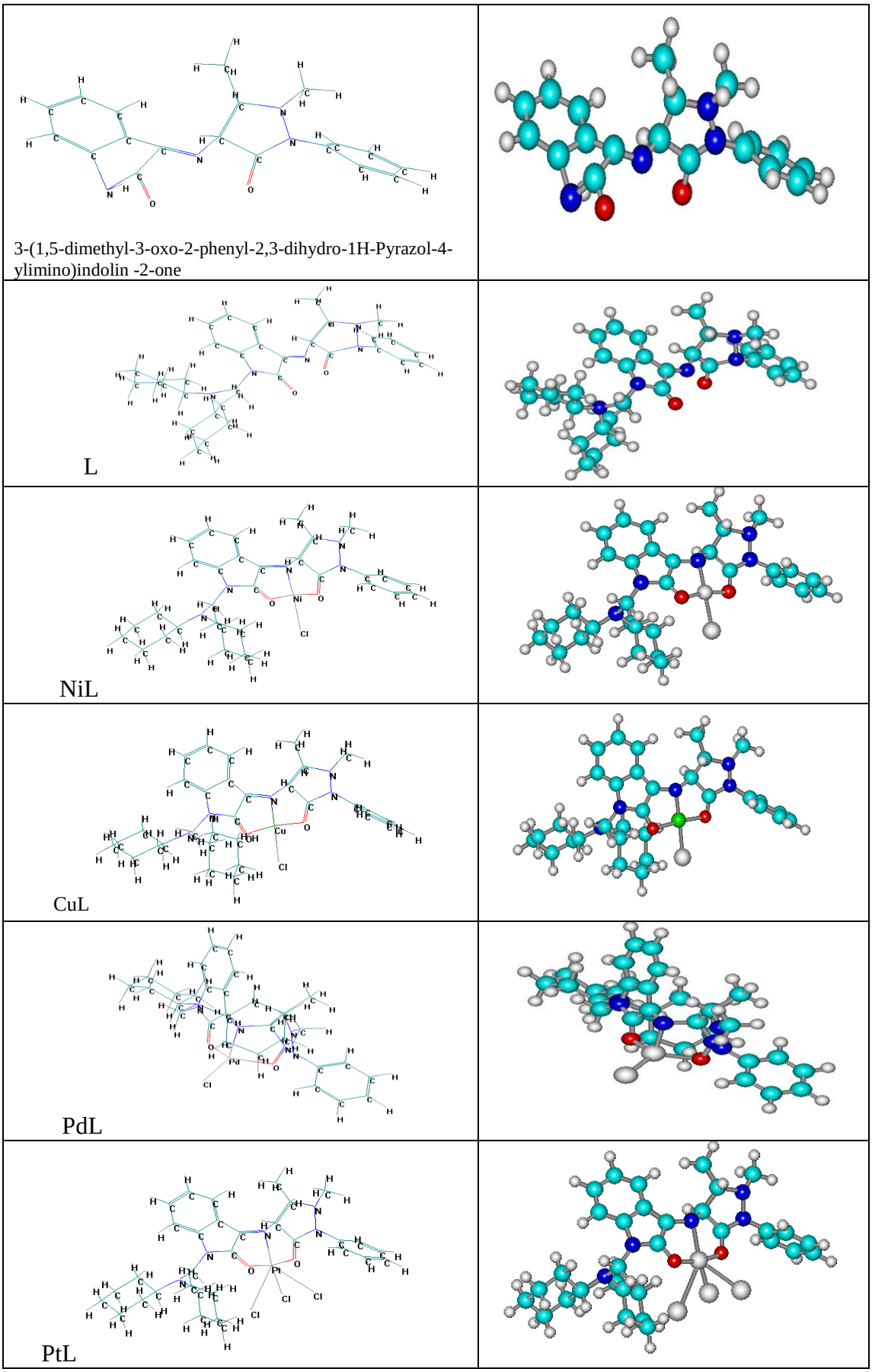


Fig. (6): The Most Probable Model Building Stable Structure of Ligand and its Metal Complexes

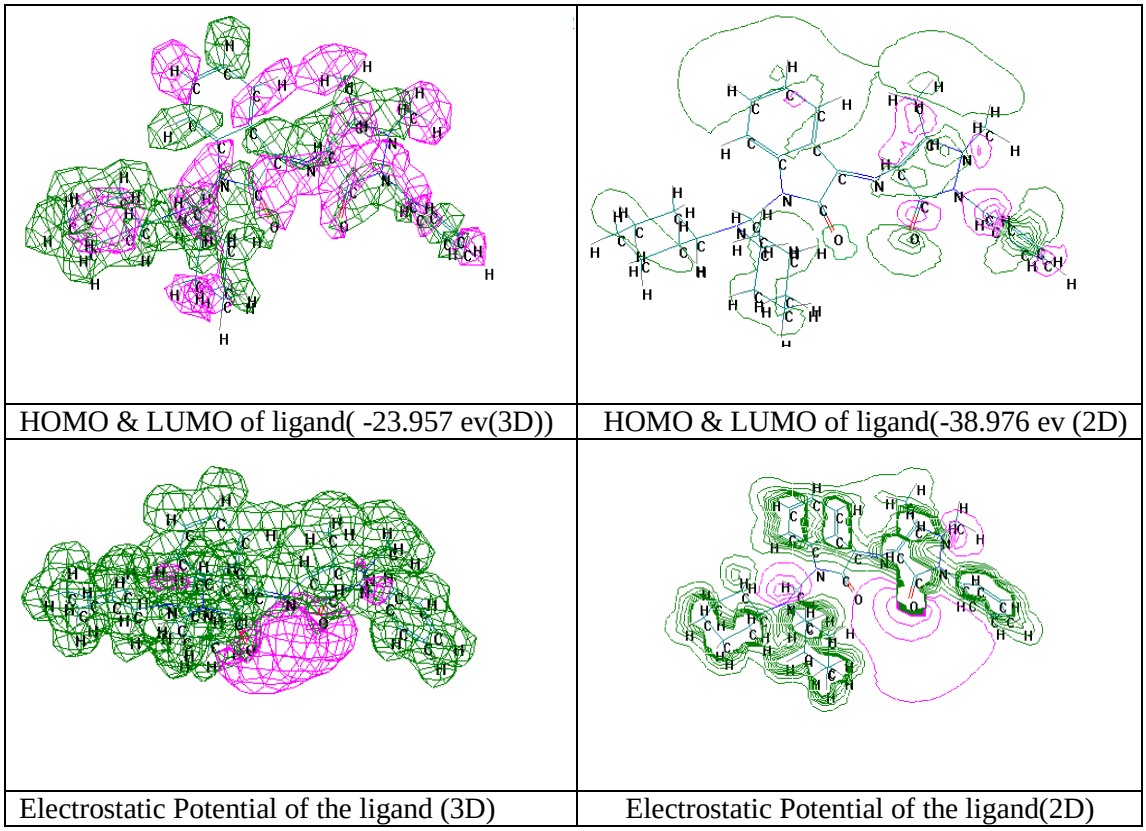
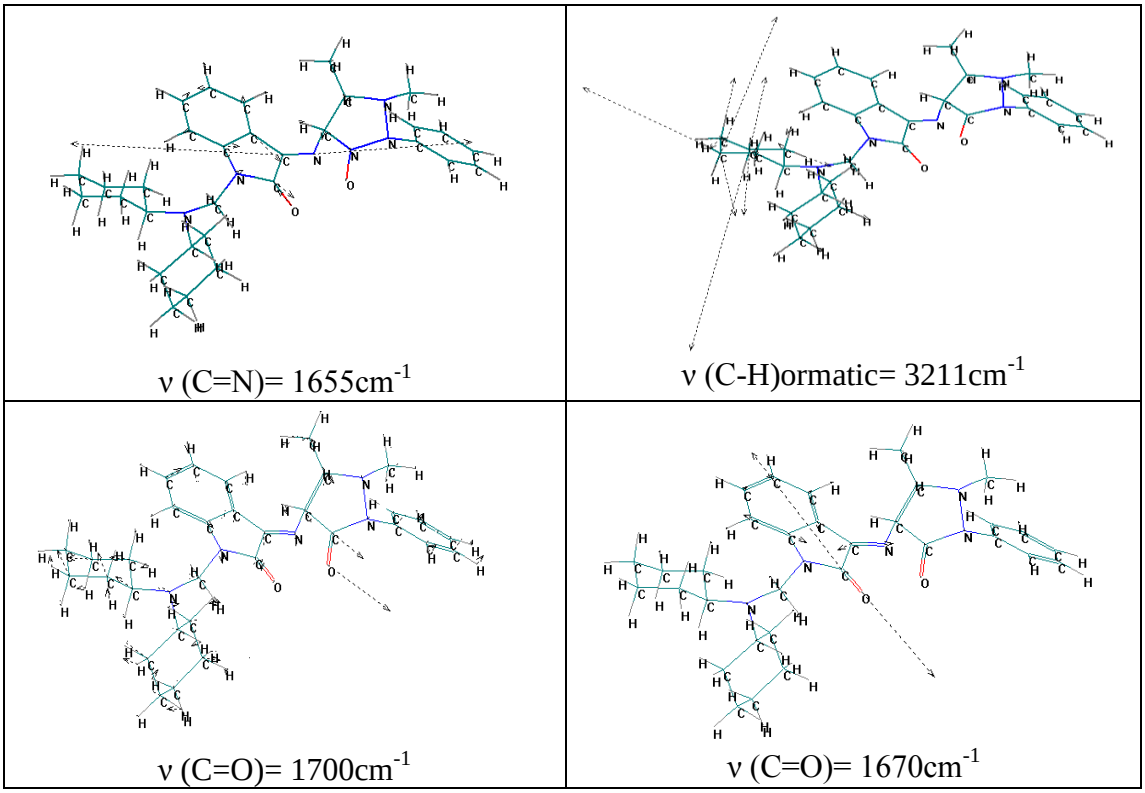


Fig. (7): HOMO, LUMO & Electrostatic Potential as 2&3D Counters for Ligand



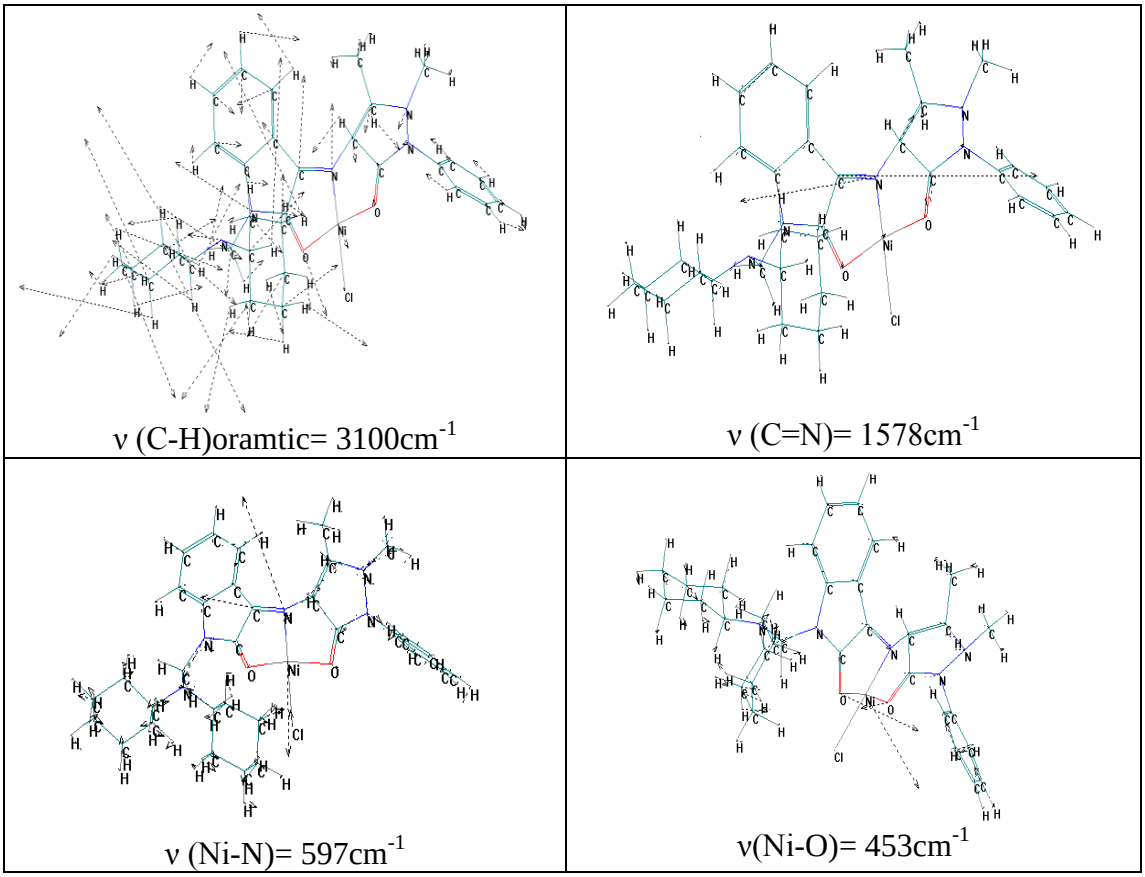


Fig. (8): Calculated Vibration Frequencies of Ligand and Complex of Nickel.

Table (4): Comparison of Experimental and Theoretical Vibrational Frequencies (cm^{-1}) for Ligand and NiL Complex

COMP.	*ν C-H ormatic*	*ν C-H alp.*	*ν C=O*	*ν C=N_{iso}*	*ν M-O*	*ν M-N*
L	(3151, 3089)* (3211, 3009)** (-1.90, 2.58)***	(2966, 2897)* (2977, 2900)** (-0.37- 0.10,)***	(1724)* (1700)** (1.39)*** (1651)* (1670)** (-1.15)***	(1620)* (1655)** (-2.16)***		
NiL	(3097, 3019)* (3100, 2998)** (-0.67, 0.69)***	(2950, 2887)* (2976, 2993)** (-0.88- 3.67)***	(1707)* (1743)** (-1.58)*** (1637)* (1702)** (-3.97)***	(1588)* (1578)** (0.62)***	(430)* (453)** (-5.34)***	(568)* (597)** (-5.10)***

*: Experimental frequency, **: Theoretical frequency, ***: Error % due to main difference in the experimental measurements and theoretical treatments of vibrational spectrum

Table(5):The Calculated Energies(in KJmol^{-1}) and Dipole Moment (in Debye) for Ligand and its Complexes

-Conformation	PM3			ZINDO/1			AMBER
	ΔH_f°	ΔE_b	μ	ΔH_f°	ΔE_b	μ	$\Delta Hf^0=\Delta Eb$
L	65.6729886	-8165.21701	2.591	-	-	-	
NiL				-16773.32308	-25193.89308	6.34	
CuL				-17516.46833	-24914.93833	8.34	
ZnL				-16899.28900	-25248.22900	7.56	
CdL	-66.7374538	-2142.497546	5.536	-18322.545620	-244667.035620	4.09	
HgL							140270920
PdL							96.113350
PtL	-	-	-	-	-	-	509.39704

Conclusion:

The ligand 1-((dicyclohexylamino) methyl)-3-(1,5-dimethyl-3-oxo-2-phenyl 1,-2,3-dihydro-1H-pyrzol-4-ylimino)indolin-2-one has been synthesized and characterized successfully . The ligand acts as a tridentate ligand for the complexation reaction with all metal ions through the O,O carbonyl group and N azomethine group atoms. All the complexes exhibit tetrahedral geometry except palladium complex square planar geometry and platinum complex octahedral geometry. The structure geometries of these compounds are also suggested in gas phase by using theoretical treatment, using Hyper chem.-6 program.

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تحضير، دراسة طيفية ومعالجة نظرية لبعض أيونات معقدات جديدة مع ليكاند ثلاثي السن (قاعدة شف و مانخ)

شيماء رجب باقر

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الخلاصة:

حضرت وشخصت معقدات أيونات المعادن الجديدة مع ليكاند ثلاثي السن 1-((dicyclohexylamino) methyl) -3- (1,5-dimethyl-3-oxo-2-phenyl,-2,3-dihydro-1H-pyrzol-4-ylimino)indolin-2-one بتحاليل كيميائية – فيزيائية . يسلك الليكاند سلوك ثلاثي السن عند تناسقه مع جميع الايونات الفلزية . أن المعقدات الجديدة التي تمتلك الصيغة التالية [M(L)Cl]Cl عندما M= [Ni(II),Cu(II),Zn(II),Pd(II),Cd(II),Pt(IV),Hg(II)] تظهر بان جميعها رباعية السطوح ماعدا البلاديوم يكون بشكل مربع مستوي والبلاتين بشكل ثماني السطوح . اقترح الشكل الهندسي للمركبات المحضرة بطريقة أخرى نظريا باستخدام إحدى برامج الحساب الجزيئية Hyper-Chem-6 بالاضافة لذلك تم مقارنة النتائج العملية مع النتائج النظرية ،أظهرت المقارنة مدى تقارب النتائج العملية من نظيرتها النظرية .

الكلمات المفتاحية: الدراسة النظرية، قاعدة مانخ، ليكاند ثلاثي السن، معقد داي سايكلوهكسايل امين.