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Synthesis, Spectral, Thermal and Theoretical Studies of Schiff base Complexes with new ligand derived from 5,5-Dimethyl-cyclohexane-1,3-dione.

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ABSTRACT

The new tetradentate Schiff base ligand L 4,4'-(1Z,1'Z)-(5,5-dimethylcyclohexane-1,3-diyldiene) bis (azan-1-yl-1-ylidene) bis (1-phenyl-1H-pyrazol-5(4H)-one) has been synthesized from condensation of 5,5-Dimethyl-cyclohexane-1,3-dione with 5-amino-2-phenyl-2,4-dihydro-pyrazol-3-one. Monomeric complexes with the general formula $[M(L)(H_2O)_2]2Cl$ where M = Co(II), Ni(II), Cu(II), Zn(II), Cd(II) and Hg(II) are reported. The structures of new ligand, mode of bonding and overall geometry of the complexes were determined through IR, UV-Vis, and NMR spectral studies, TGA curve, magnetic moment measurements, elemental microanalyses (C.H.N.O.), chloride containing, Atomic absorption and conductance. These studies revealed octahedral geometries for all complexes. Complex formation studies via molar ratio and continuous variation methods in DMF solution were consistent to those found in the solid complexes with a ratio of (M : L) as (1 : 1). Hyper Chem-8 program has been used to predict structural geometries of compounds in gas phase, the heat of formation, (binding, total and electronic energy) and dipole moment at 298 K.

Keywords: Schiff base Complexes, 5,5-Dimethyl-cyclohexane-1,3-dione Theoretical Studies.

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INTRODUCTION

Schiff base derivatives attract a significant interest and occupy an important role in the development of coordination chemistry [1]. The coordination chemistry of transition metals with ligands from the 5, 5-dimethyl cyclohexane-1,3- dione has been of interest due to different bonding modes show by these ligands with both electron rich and electron poor metals. Schiff bases play an important role in inorganic chemistry as they easily form stable complexes with most transition metal ions. The presence of donor atoms in the ligand will play an important role in the formation of a stable chelating and this situation facilitates the complexation process [2]. Moreover, Schiff base complexes containing metal ions have been studied in several research areas such as structural chemistry [3]. Metal complex with Schiff bases are important class of ligands due to their synthetic flexibility, selectivity and sensitivity towards the central metal atom, structural similarities with natural biological substances, and also, due to presence of azomethine group which imports in elucidating the mechanism of transformation and racemisation reaction in biological system [4,5] also have been studied for their application in clinical, analytical and pharmacological areas [6].

EXPERIMENTAL

Instrumentation

Elemental (C.H.N.O) analyses were carried out on a Perkin-Elmer automatic equipment model 240.B. Electronic absorption spectra were recorded in the range (200-1100) nm on a Shimadzu 160 Spectrophotometer. Thermal analysis studies of the compounds were performed on Perkin-Elmer Pyris Diamond DTA/TG Thermal system under nitrogen atmosphere at a heating rate of 10°C/min. (FT-IR) the spectra were recorded in the range (4000-400) cm^{-1} on a Shimadzu 3800, spectrometer. $^1\text{H-NMR}$ spectra were recorded using Bruker 400 MHz spectrometer and Mass spectra were obtained by LC-Mass 100P Shimadzu. Melting points were obtained on a Buchi SMP-20 capillary melting point apparatus and are uncorrected. Metals were identified using a Shimadzu (F.A.A) 680 G atomic absorption Spectrometer. Conductivity measurements were made with DMSO solutions using a Jenway 4071 digital conductivity meter at room temperature, chlorine content. Magnetic properties were measured using (Balance magnetic susceptibility model MSR-MKi).

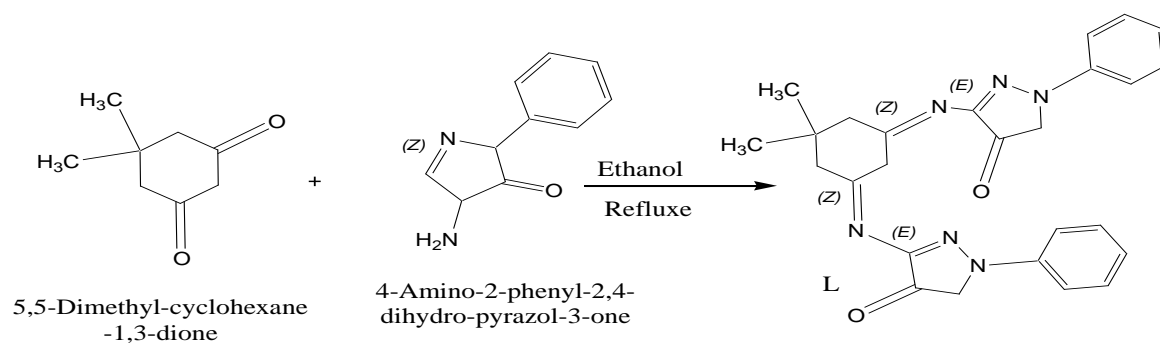
Materials

The following chemicals were commercially available products of analytical reagent grade. 5,5-Dimethyl-cyclohexane-1,3-dione, 5-amino-2-phenyl-2,4-dihydro-pyrazol-3-one, DMSO, pure ethanol, methanol, CaCl_2 , $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$, CuCl_2 , $\text{ZnCl}_2 \cdot 2\text{H}_2\text{O}$, $\text{CdCl}_2 \cdot \text{H}_2\text{O}$ and HgCl_2 were obtained from Fluka, Aldrich.

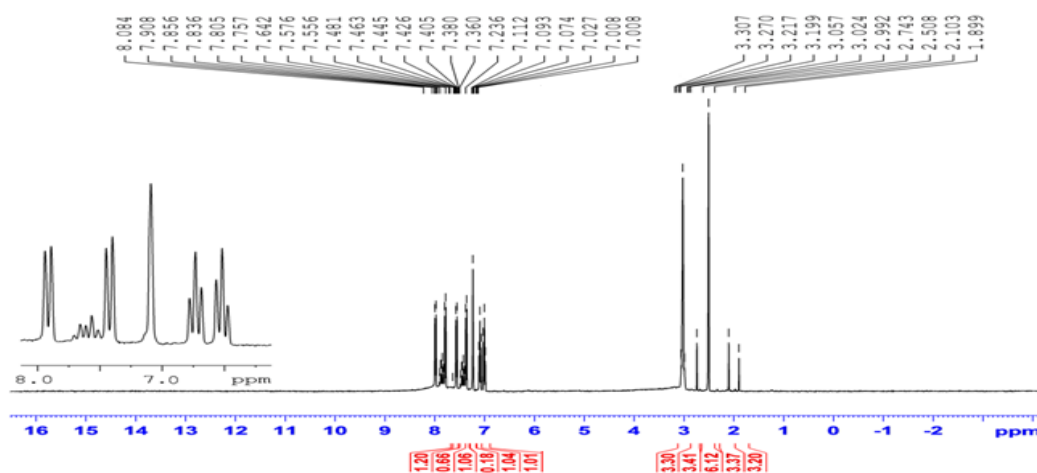
Synthesis of Ligand: 4,4'-(1Z,1'Z)-(5,5-dimethylcyclohexane-1,3-diyldene) bis(azan-1-yl-1-ylidene) bis(1-phenyl-1H-pyrazol-5(4H)-one).

An ethanolic solution (15 ml) of 5,5-Dimethyl-cyclohexane-1,3-dione(1.4 g, 0.01mol) was added to a mixture containing an neutral ethanolic solution by (NaOH + glacial acetic acid) (15 ml) of 4-amino-1-phenyl-1H-pyrazol-5(4H)-one (3.5g, 0.02mol). The resulting mixture was refluxed for 2 hours with stirring. A light red crystals glossy was formed and then re-crystallized from a mixture of ethanol. The product was dried over anhydrous CaCl_2 in vacuum. Yield: 88% (4.03 g), mp191-192 °C.

The singlet signal observed at ($\delta=1.899$ ppm, 2.103 ppm) in the spectrum of free Schiff base [L], was assigned to the methyl group (C- CH_3), singlet signal showed at ($\delta=2.743$ ppm, 3.024 ppm), was attributed to the (-C-H), singlet signal showed at ($\delta=3.199$ ppm, 3.307 ppm), was attributed to the (-C-H), multiple a ranged between ($\delta=7.008 - 8.084$ ppm) were assigned to the aromatic protons. The singlet signal appeared at ($\delta=2.50$ ppm) can be assigned to the solvent (DMSO).The molecular ion peak for the free ligand show Figure 1, was observed at $m/z = 454$ (M) (relative abundance is 10%) for $\text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_6$ which is in excellent agreement with the (454.52) theoretical value [7].



Scheme 1: Preparation of the Ligand


 Figure 1: ¹H-NMR Spectrum of free Ligand

Synthesis of Complexes

A solution of the ligand (1 mol) in methanol (25 ml), and methanol solution (30 ml) of the metal salt (1 mol) ($\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$, CuCl_2 , $\text{ZnCl}_2 \cdot 2\text{H}_2\text{O}$, $\text{CdCl}_2 \cdot \text{H}_2\text{O}$ and HgCl_2) was then added drop wise. The resulting mixture was refluxed 6 hrs in (40-50) °C, resulting in the formation of a solid mass which was washed several times with hot ethanol and dried under vacuum. Physical properties for the complexes are given in Table 1.

Programs used in Theoretical Calculation

Hyper Chem-8 program is a sophisticated molecular modeler, editor and powerful computational package that are known for its quality, flexibility and ease of use, uniting 2D visualization and animation with quantum chemical calculations, molecular mechanics and dynamic. (PM3) and (AMBER) are more popular than other semi-empirical methods due to the availability of algorithms and more accurate than with other methods. It has parameterized primarily for organic molecules and selected transition metals [8].

RESULTS AND DISCUSSION

Tetradentate complexes were obtained upon reaction between metal ions and Schiff base with molar ratio (1:1) (M:L). The synthesized Schiff base ligand and its complexes are very stable at room temperature in the solid state. The ligand and its metals complexes are generally soluble in hot DMF and DMSO. The yields, melting/decomposition points, elemental analyses of Schiff base and its metals complexes are presented in Table 1. It is found that the analytical data are in a good agreement with the proposed stoichiometry of the complexes. Schiff base was decomposed at temperatures higher than 390°C, while all complexes were decomposed at temperatures higher than (265-293) °C. The ligand and its metal complexes have dye character due to the high molar extinction constant. Molar conductance values were found in the range (109-146) S.

$\text{cm}^2 \text{mol}^{-1}$ for all complexes which indicate that they are electrolytes [1:2] [9]. These were determined in (DMSO) solution (10^{-3}M). Physical properties and elemental microanalysis are listed in Table 1.

Table 1: Microanalysis results and some physical properties of the Ligand and its complexes

Sam.	Molecular Formula = M_{wt}	m.p. °C	Element analysis % Calcu (Found)				
			M	C	H	N	Cl
L	$\text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_2$ 545.52	191-192		68.70 (67.97)	5.77 (5.01)	18.49 (20.01)	
LC ₁	$\text{C}_{26}\text{H}_{30}\text{N}_6\text{O}_4\text{CoCl}_2$ 620.39	300 d	9.50 (9.99)	50.34 (51.09)	4.87 (4.11)	13.55 (14.18)	11.43 (10.77)
LC ₂	$\text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_4\text{NiCl}_2$ 620.15	281 d	9.46 (9.99)	50.36 (49.79)	4.88 (5.11)	13.55 (14.18)	11.43 (12.11)
LC ₃	$\text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_4\text{CuCl}_2$ 625.01	267 d	10.17 (10.99)	49.96 (49.09)	4.84 (5.11)	13.45 (15.18)	11.34 (11.09)
LC ₄	$\text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_4\text{ZnCl}_2$ 626.85	265 d	10.43 (10.99)	49.82 (49.09)	4.82 (5.11)	13.41 (15.28)	11.31 (12.01)
LC ₅	$\text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_4\text{CdCl}_2$ 673.87	293 d	16.68 (15.99)	46.34 (47.09)	4.49 (5.11)	12.47 (13.28)	10.52 (10.01)
LC ₆	$\text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_4\text{HgCl}_2$ 762.05	278 d	26.32 (25.99)	40.98 (40.09)	3.97 (4.11)	11.03 (12.18)	9.30 (10.01)

d = decompose

Mass spectra for complexes

The LC-Mass spectra of complexes [LC₃, LC₄] Figure 2 and Figure 3 showed the parent ion peaks at ($M/Z=625.01$) and ($M/Z=626.85$) correspond to ($M= \text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_6\text{Cu}$) and ($M= \text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_6\text{Zn}$) respectively. The fragmentation pattern is shown in Table 2.

Table 2: The Fragmentation Pattern data for Complexes

Complex	Peaks
LC ₃ $\text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_6\text{Cu}$	625, 355, 212, 67
LC ₄ $\text{C}_{26}\text{H}_{26}\text{N}_6\text{O}_6\text{Zn}$	626, 355, 212

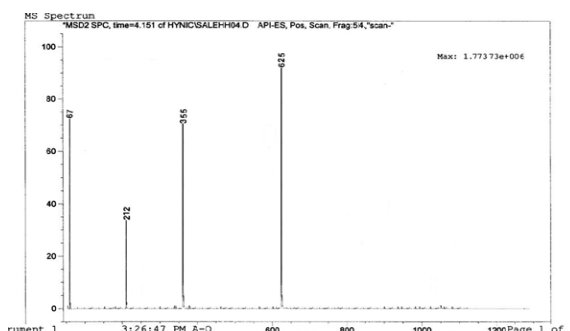


Figure 2: LC-Mass Spectrum of LC₃

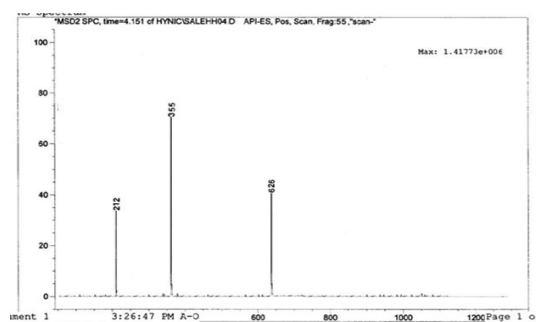


Figure 3: LC-Mass Spectrum of LC₄

IR spectra

The characteristic stretching vibration modes concerning Schiff base (L) and its metal complexes are described in Table 3. The ligand (L) exhibited a strong high intensity bands appeared at $(1740) \text{cm}^{-1}$, $(1680) \text{cm}^{-1}$ and $(1620) \text{cm}^{-1}$ which were ascribed to the stretching mode of $\nu(\text{C}=\text{O})$, $\nu(\text{C}=\text{N})$ azomethen group and $\nu(\text{C}=\text{N})$ ring, as show in Table 3, respectively. The weak absorption bands appeared at (3019) and $(2955) \text{cm}^{-1}$ were assigned to $\nu(\text{C}-\text{H})$ aromatic and $\nu(\text{C}-\text{H})$ aliphatic, respectively. Pertaining to the complexes, the Schiff base behaved as a tetra dentate ligand, which were been coordinating with the metal via oxygen of carbonyl group

and nitrogen of the azomethene group. The mentioned coordination was confirmed by shifting the bands $\nu(\text{C}=\text{O})$ and $\nu(\text{C}=\text{N})$ to lower frequencies about $(13-25) \text{ cm}^{-1}$ and $(13-31) \text{ cm}^{-1}$, respectively [10, 11].

These observations were further indicated by the appearance of $\nu(\text{M}-\text{N})$. the spectra showed new bands at $[(563), (578), (513), (575,559), (561) \text{ and } (569, 519)] \text{ cm}^{-1}$ can be refer to $\nu(\text{M}-\text{N})$ for complexes with metals Co(II), Ni(II), Cu(II), Zn(II), Cd(II) and Hg(II), respectively.

Abroad band was observed round $(3406, 3406, 3431, 3377, 3469 \text{ and } 3449) \text{ cm}^{-1}$ and $(725, 754, 756, 760, 760 \text{ and } 760) \text{ cm}^{-1}$ in each of Co(II), Ni(II), Cu(II), Zn(II), Cd(II) and Hg(II) complexes spectra respectively, which is assigned to the $\nu(\text{O}-\text{H})$ and $\delta(\text{H}_2\text{O})$. The results led to a suggestion for the presence of water molecules. The new bands supported the coordination of the ligand to the central metal ion through oxygen atom of molecular water, and the spectra showed bands at $[(470, 438), (466), (467, 428), (476), (472) \text{ and } (465, 438)] \text{ cm}^{-1}$ can be refer to $\nu(\text{M}-\text{O})$ for complexes with metals Co(II), Ni(II), Cu(II), Zn(II), Cd(II) and Hg(II), respectively [12-15].

Table 3 Infrared Spectra Data of the Free Ligand (L) and its Complexes in (cm^{-1})

Comp.	$\nu\text{C}=\text{O}$	$\nu\text{C}=\text{N}$	$\nu\text{C}=\text{N}$ ring	$\nu(\text{OH}_2)$ $\delta(\text{OH}_2)$	$\nu\text{M}-\text{N}$	$\nu\text{M}-\text{O}$	Other bands
L	1740	1680	1620	-			ν C-H arom =3019 ν C-H aliph=2955
LC ₁	1723	1649	1612	3406 725	563	470 438	ν C-H arom =3087 ν C-H aliph=2983
LC ₂	1726	1654	1614	3406 754	578	466	ν C-H arom =3046 ν C-H aliph=2987
LC ₃	1724	1657	1617	3431 756	513	467 428	ν C-H arom =3068 ν C-H aliph=2971
LC ₄	1727	1667	1614	3377 760	575 559	476	ν C-H arom = ν C-H aliph=2959
LC ₅	1716	1663	1618	3469 760	561	472	ν C-H arom =3077 ν C-H aliph=2957
LC ₆	1715	1660	1609	3449 760	569 519	465 438	ν C-H arom =3029 ν C-H aliph=2986

UV-Vis Spectra, Magnetic Moments

The electronic spectrum of LC₁ Co(II) complex, displayed four new absorption peaks. The first peak at (392) nm attributed to the (C. T), and the second, third and four peaks at (585)nm, (698)nm and (823) nm due to (d-d) electronic transitions type ${}^4\text{T}_{1g} \rightarrow {}^4\text{T}_{2g}(\text{p})$, ${}^4\text{T}_{1g} \rightarrow {}^4\text{A}_{2g}(\text{F})$ and ${}^4\text{T}_{1g} \rightarrow {}^4\text{T}_{2g}(\text{F})$, which are a good evidence for octahedral geometry. The electronic spectrum of LC₂ Ni(II) complex displayed third new absorption peaks. The first peak at (392) nm attributed to the (C. T), and the second and third peaks at (506)nm and (717) nm due to (d-d) electronic transitions type ${}^3\text{A}_{2g} \rightarrow {}^3\text{T}_{1g}(\text{p})$, ${}^3\text{A}_{2g} \rightarrow {}^3\text{T}_{1g}$ and ${}^3\text{A}_{2g} \rightarrow {}^3\text{T}_{2g}$, which are a good evidence for octahedral geometry. The electronic spectrum of LC₃ Cu(II) complex displayed second new absorption peaks. The first peak at (397) nm attributed to the (C. T), and the second and third peaks at (618)nm due to (d-d) electronic transitions type ${}^2\text{B}_{1g} \rightarrow {}^2\text{A}_{1g}$ which are a good evidence for distorted octahedral geometry [15-18]. The electronic spectrum of LC₄ Zn(II) displayed first new absorption peak. The first peak at (400)nm attributed to the (C. T) which are a good evidence for octahedral geometry. The electronic spectrum of LC₅ Cd (II) complex displayed first new absorption peak. The first peak at (402)nm attributed to the (C. T) which is a good evidence for octahedral geometry. The electronic spectrum of LC₆ Hg(II) complex displayed first new absorption peak. The first peak at (404)nm attributed to the (C. T) which is a good evidence for octahedral geometry [16-17].

A similar method to that mentioned in measurement the magnetic susceptibility and μ_{eff} of ligand complexes. The μ_{eff} values were listed in Table 4. LC₁= 4.39) B.M, LC₂= 4.24) B.M, LC₃=1.9) B.M, but LC₄, LC₅ and LC₆] diamagnetic [17].

Table 4: Electronic Spectral Data of the Metal Complexes with Ligand and Magnetic Moments,

Complexes	λ nm	ϵ cm^{-1}	ABS	ϵ L. $\text{mol}^{-1}\text{cm}^{-1}$	Assignment	Λ $\text{S.cm}^2\text{mol}^{-1}$	μ_{eff} B.M
LC ₁	274	36496	2.072	20720	L.F.	130	4.39
	345	28985.5	2.217	22170	L.F.		
	392	25510	2.421	2421	C.T.		
	585	17094	0.621	621	${}^4\text{T}_{1g} \rightarrow {}^4\text{T}_{1g}(\text{p})$		
	698	14326.6	0.465	465	${}^4\text{T}_{1g} \rightarrow {}^4\text{A}_{2g}(\text{F})$		
	823	12150.6	0.248	248	${}^4\text{T}_{1g} \rightarrow {}^4\text{T}_{2g}(\text{F})$		
LC ₂	274	36496	2.072	20720	L.F.	146	3.24
	345	28985.5	2.217	22170	L. F.		
	392	25510	2.421	242	C.T.		
	506	19762.8	0.301	301	${}^3\text{A}_{1g} \rightarrow {}^3\text{T}_{2g}(\text{p})$		
	717	13947	0.018	180	${}^3\text{A}_{1g} \rightarrow {}^3\text{T}_{1g}(\text{F})$ ${}^3\text{A}_{1g} \rightarrow {}^3\text{T}_{2g}(\text{F})$		
LC ₃	289		1.008	1008	L.F	142	1.9
	333		1.410	1410	L.F		
	397		1.521	1521	C.T		
	618		0.009	9	${}^2\text{B}_{1g} \rightarrow {}^2\text{A}_{1g}$		
LC ₄	280		1.683	1683	L.F	121	dia
	325		1.230	1230	L.F.		
	400		2.254	2254	C.T		
LC ₅	281		1.243	1243	L.F	109	dia
	327		1.233	1233	L.F.		
	402		2.255	2255	C.T		
LC ₆	290		1.003	1003	L.F	132	dia
	332		1.314	1314	L.F.		
	404		2.246	2246	C.T		

Thermal Gravimetric Analyses TGA

To understand the thermal decomposition processes of the studied compounds, the Schiff base ligand and its metal complexes were examined by thermo gravimetric analysis in the temperature range of 30–700 °C.

TG curve of L show relatively rapid decomposition in the first (33.2- 121.7 °C), second (121.7- 429) and third (460.3 - 689°C) steps with T_{DTG} peaks at 68.7°C, 368 °C and 654°C. The very large and strongly sharp T_{DTG} peak observed for the first step at 368 °C is preceded with a sharp peak. 5.27%, 28.82% and 64.09% mass losses in the first, second and third steps correspond to the release of (OH), (C₇H₉N₂O₂) and (C₁₈H₁₆N₄O₄) fragments (cal. 4.756 %, 28.788% and 64.352 %, respectively), Show Figure 4 and the Table 5 Characterization Parameters of thermal decomposition (10°C min⁻¹) of ligand [15].

The TG curve of Co(II) complexes with L show relatively rapid decomposition in the first (35.100°C) and second (100.599.6°C) steps with T_{DTG} peaks at 80.3°C and 309.6°C. The very large and strongly sharp T_{DTG} peak observed for the first step at 309.6°C is preceded with a sharp peak. 12.24 % and 86.49% mass losses in the first and second steps correspond to the release of (2H₂O) and (C₂₆H₂₂N₆O₃) fragments and final product (CoO) (cal. 2.31%, 50.95% and 42.03%, respectively). The tentative decomposition reaction of L₄C₁ is shown in Table 5.

The TG curve of Zn (II) complexes with L show relatively rapid decomposition in the first (83-231°C), second (231- 396°C) and third (396- 599.6°C) steps with T_{DTG} peaks at 190.5°C, 358°C and 482°C. The very large and strongly sharp T_{DTG} peak observed for the first step at 358°C is preceded with a sharp peak. 8.36 %, 40.60% and 43.38% mass losses in the first, second and third steps correspond to the release of (2H₂O), (C₁₀H₁₂N₂O) and (C₁₆H₁₀N₄O₂) fragments and final product (ZnO) (cal. 10.05%, 40.46% and 42.96%, respectively). The tentative decomposition reaction of LC₄ is shown in Table 5

The TG curve of Hg (II) complexes with L show relatively rapid decomposition in the first (80-205°C) and second (255-520°C) steps with T_{DTG} peaks at 165°C and 360°C. The very large and strongly sharp T_{DTG} peak

observed for the first step at 360°C is preceded with a sharp peak. 10.23 % and 78.39% mass losses in the first and second steps correspond to the release of (2H₂O) and (C₂₆H₂₂N₆O₃) fragments and final product (HgO) (cal. 11.09% and 79.68%, respectively). The tentative decomposition reaction of LC₆ is shown in Table 5. [7,15,17].

Table 5: Characterization Parameters of Thermal Decomposition (10°C min⁻¹) for Metal Complexes of Ligand

Com	TG range (°C)	DTG _{max} (°C)	%Estimated (calculated)		Assignment
			Mass Loss	Total mass Loss	
L	33.2-121.7	(98.188)	4.756 (5.27)	68.7	-OH
	122.1-429	97.896	28.788(28.82)	368	-C ₇ H ₉ N ₂
	460.3-689		64.352 (64.09)	654	-C ₁₈ H ₁₆ N ₄ O C
LC ₁	35-100	80.3	(13.08) 12.24	98.73	2H ₂ O
	100- 599.6	309.6	(85.07) 86.49	(98.15)	C ₂₆ H ₂₂ N ₆ O ₃ CoO
LC ₄	83-231	190.5	(10.05) 8.36	92.34	2H ₂ O
	231-396	358	(40.46) 40.60	(93.47)	C ₁₀ H ₁₂ N ₂ O
	396-599.6	482	(42.96) 43.38		C ₁₆ H ₁₀ N ₄ O ₂ ZnO
LC ₆	80-205	165	(11.09) 10.23	88.62	2H ₂ O
	255-520	360	(79.68) 78.39	(90.77)	C ₂₆ H ₂₂ N ₆ O ₃ HgO

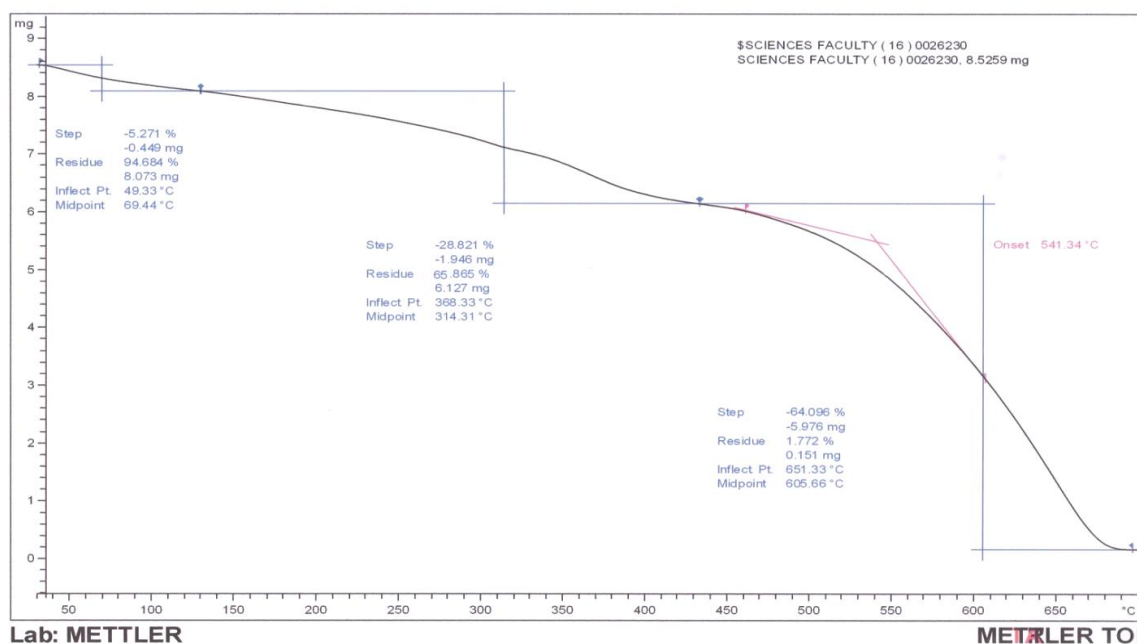


Figure 4: TGA and DTA Curve of Ligand L

Electrostatic Potentials:

Electron distribution governs the electrostatic potential of the molecules. The electrostatic potential (E.P) describes the interaction of energy of the molecular system with a positive point charge. (E.P) is useful for finding sites of reaction in a molecule; positively charged species tend to attack a molecule where the electrostatic potential is strongly negative (electrophilic attack) [19]. The (E.P) of the free ligand was calculated and plotted as 2D contour to investigate the reactive sites of the molecules, Figure 5. Also one can interpret the stereochemistry and rates of many reactions involving "soft" electrophiles and nucleophiles in terms of the properties of frontier orbital HOMO and LUMO. The results of calculations show that the LUMO of transition metal ions prefer to react with the HOMO of three-donor atoms of two oxygen of carbonyl and nitrogen of azomethen group for free ligand, Figure 6.

All theoretically probable structures of free ligand and their complexes have been calculated by (PM3) and (ZINDO/1) methods in gas phase to search for the most probable model building stable structure, Table 6. [7, 11].

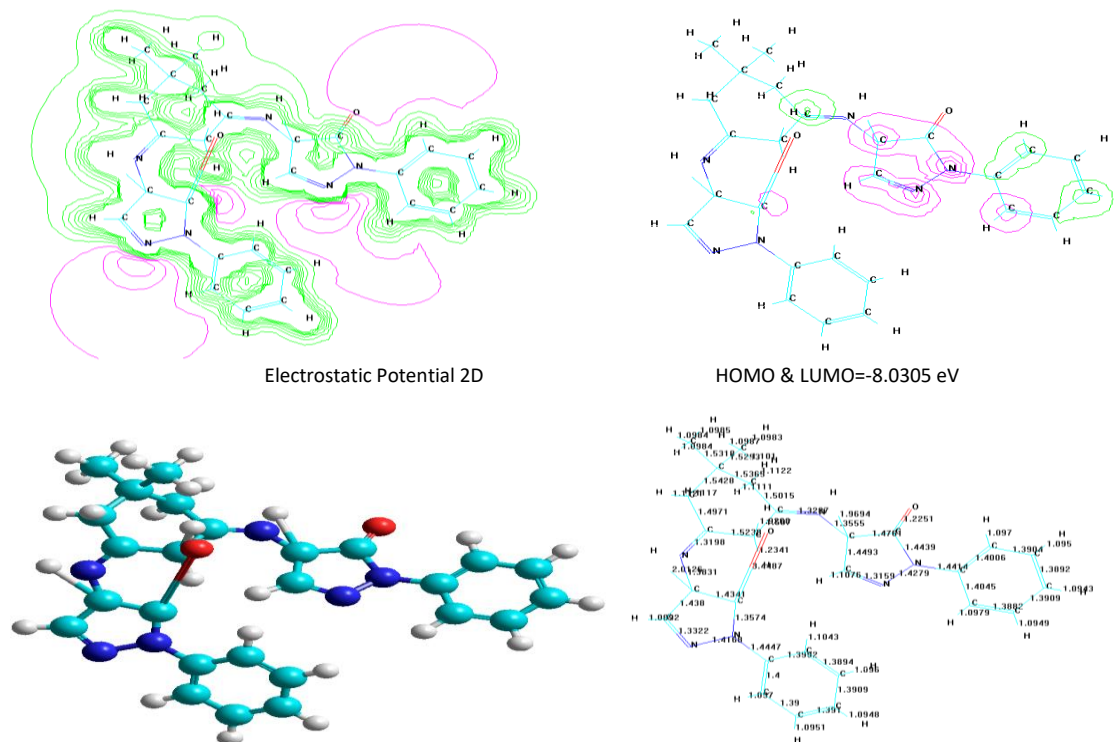
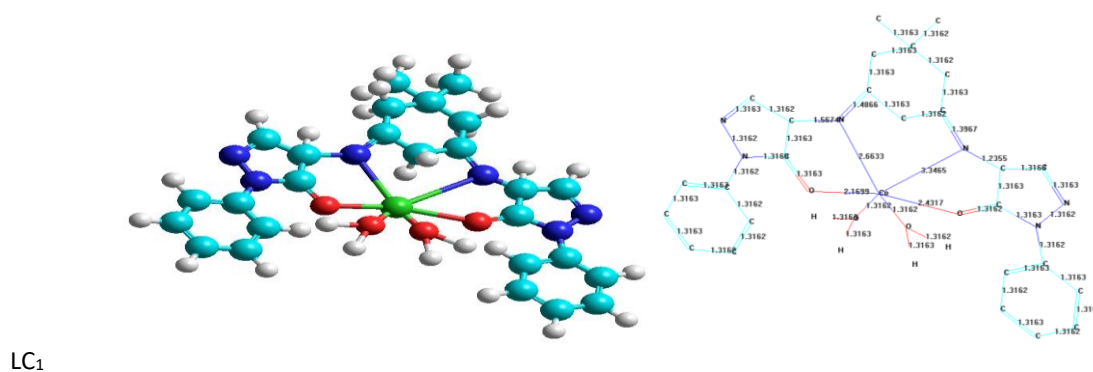


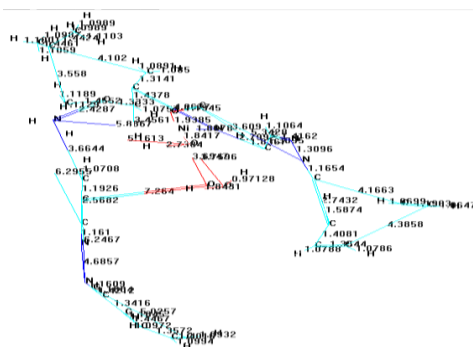
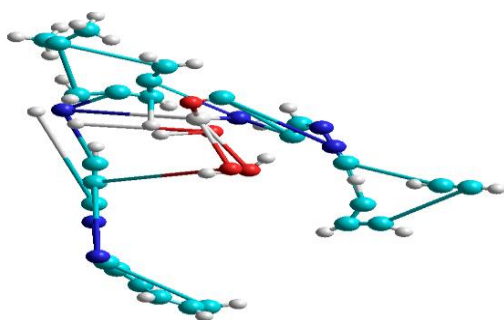
Figure 5: Electrostatic Potential (HOMO and LUMO) Contours for Ligand

Table 6: Conformation Energetic in (K J.Mol⁻¹) for the Ligand and Complexes

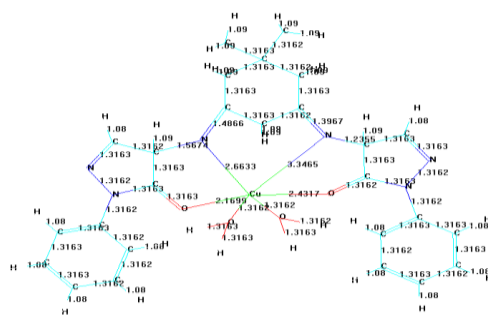
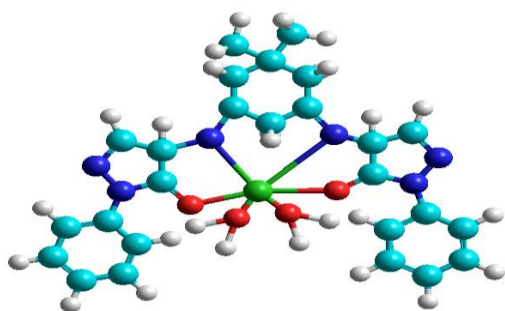
Comp.	Total energy	Binding energy	Heat of formation	Electronic energy	Dipole (Debyes)	Isolated Atomic Energy
L	-116149.7794	-6465.99042	128.919	-1121869.745	10.874	-109683.789
LC ₁	-136804.6161	-69381.3179	14.288	-1256303.654	12.750	-124866.298
LC ₂	-154545.90	-6513.5828	511.65318	-1162035.545	6.776	-148032.3179
LC ₃	-136545.6468	-9644.4574	92.6685	-1066928.336	6.115	-124901.189
LC ₄	-131804.6161	-6938.3179	15.288	-1286303.654	10.750	-124866.298
LC ₅	-131361.8681	-6609.42211	339.73388	-1065209.29	10.094	-124752.4459
LC ₆	-131545.6468	-6644.4574	292.6685	-1066928.336	2.115	-124901.189



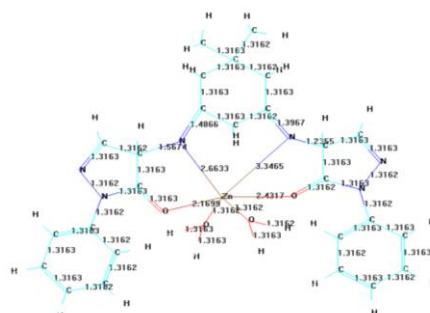
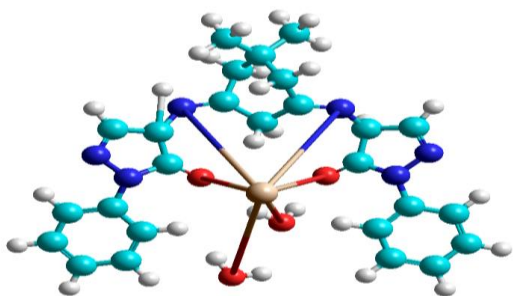
LC₁



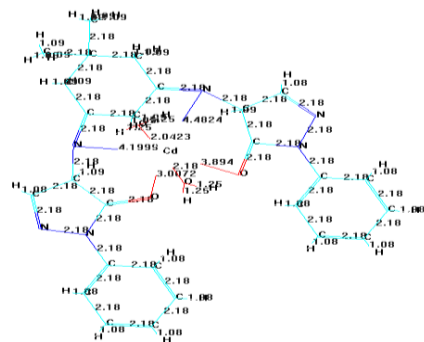
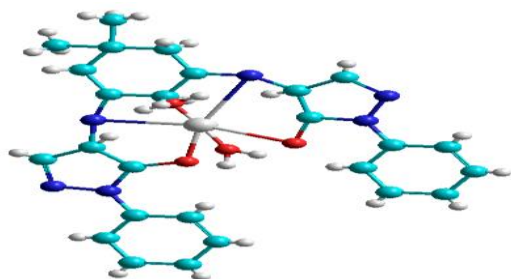
LC₂



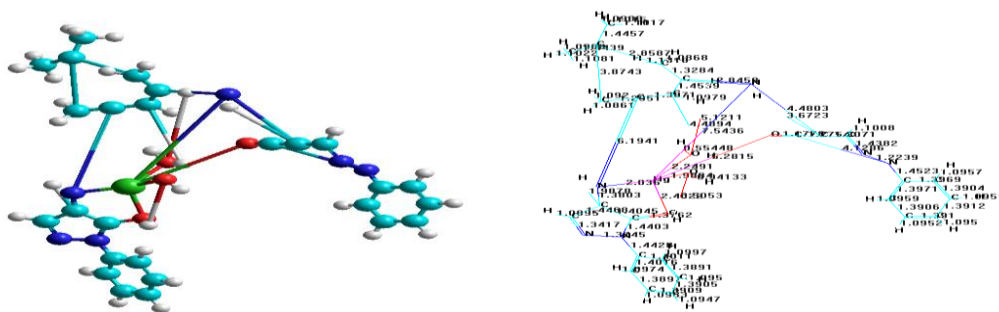
LC₃



LC₄



LC₅


 LC₆
Figure 6: Conformational Structure of metal complexes

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