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Synthesis, characterization and theoretical evaluation of the transition metal complexes of 2, 6-diacetylpyridine-derived N_5-acyclic ligands

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Abstract: A series of transition elements complexes with [2, 6-diacetimino-pheylenediamine –[2, 2ˈdiyl] pyridine]of the general formula [MLCl]Cl, M= Zn(II), Cd(II), Hg(II) and [CrLCl]Cl_2, respectively have been synthesized and fully characterized on the bases of C.H.N.M, elemental analysis, ^{13}C NMR, UV- Visible and FTIR spectra, in addition the structure of complexes was characterized by magnetic moments and molar conductance in DMSO solution, and molar ratio of metal were also determined. The obtained data of spectra in conjugation with microelemental analyses suggested the octahedral symmetry for all the complexes since the molar ratio(M: L) is 1:1, and the newly ligand behaved as neutral pentadentate through four nitrogen atoms of NH_2,C=N and pyridine ring on the basis of infrared spectroscopy and other analysis of molar conductance and magnetic moments for solid complexes. A theoretical treatment of the formation of complexes in the gas phase was studied, this was done using the HYPERCHEM-6 program for the Molecular mechanics and Semi-empirical calculations.

Keywords: Synthesis, Characterization, Theoretical Evaluation, N_5 Acyclic, Transition Metal

1. Introduction

Complexes of metal ions with synthetic macro cyclic ligand are of great importance, in part because of their research lance to many natural system e. g. , porphyrin and, calamines publication of several reviews and books covering various aspects of synthetic macro cyclic ligands is witness to the great attached to them[(1-3)].acyclic model N_2O_2, N_2S_2 and N_4 system derived from 2,6 di acetyl pyridine are used in some chemical processes as catalysts[(4-5)] .They are also used in biological models to understand the structure of bio-molecules[(6)].

In the present paper the Cr(III) , Zn(II) , Cd(II) and Hg(II) chelate with N5-macrocyclic ligand derived from 2,6-dimethylpyridine and O-phenyline di amine have prepared , fully characterized by common spectral and analytical techniques.

2. Experimental

2.1. Physical Measurements

IR spectra were recorded as KBr discs using a Shimadzu 8300 FTIR spectrophotometer in range (4000-400) cm^{-1}. Electronic spectra of the prepared compounds were measured in the region 200 in**11** for 10^{-3} M solution in DMF at 25 °C using Shimadzu 160 spectrophotometer, with 1.000 ± 0.001 Cm matched quartz cell. ^{13}C- NMR were acquired with BRUKER-400 spectrometer in DMSO-*d6* solvent. The NMR spectra were recorded at Queen Mary, University of London/ United Kingdom. Elemental microanalysis were performed on a (C.H.N) were performed by using Elemental analyzers perkin –Elmer-240B, while metal contents of the complexes were determined by atomic absorption type shimadzu (A, A-670). The chloride contents for complexes were determined by using potentiometer titration method on (686-Swiss). Electrical conductivity measurements of the complexes

were recorded at 25 °C for 10^{-3} M solution of the sample in DMSO using a PW9527 digital conductivity meter. Magnetic susceptibility measurements were obtained at 25 °C on the solid state applying Faraday, s method using Bruker BM6 instrument.

2.2. Materials

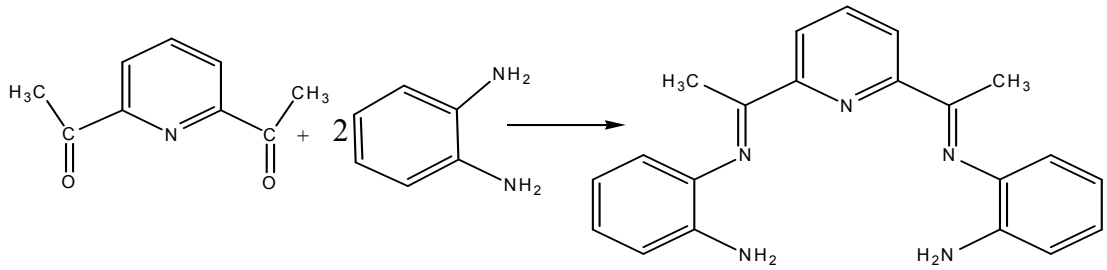
Reagents were purchased from Fluka and BDH and Redial-Dehenge Chemical Company.

A- Synthesis of N5 Acyclic macrocylic ligand (L): A 20 ml methanolic solution of 2,6-diacetyl pyridine (0.01 mole) was refluxed with 100 ml methanolic solution of re crystallized O-phenyleneiamine (0.02 mole) for about 4 hrs. A few drops of glacial acetic acid were added to the mixture and refluxed continued for (12-24) hrs. The mixture was concentrated to half of its volume and kept in desiccators for days .The ligand was filtered, washed with methanol , acetone and ether , dried in vacuum , over $CaCl_2$ pellets , in yield 80% .The physical properties and analytical data, are shown in Table (1).

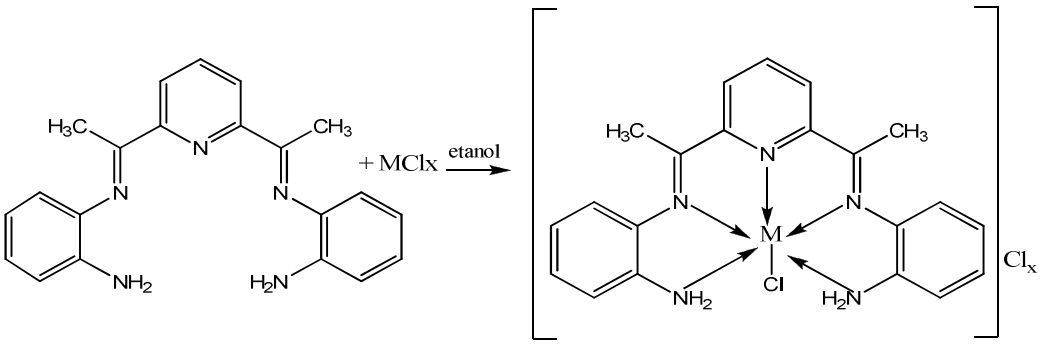
The general structure of ligand obtained from chemical analysis and spectral methods, are given in Scheme (1).The full name of the ligand will be replaced by (L) for the rest of this paper.

Table (1) *some physical and chemical properties of the prepared ligand and complexes*

coumpound	M.p.	colour	%C Calc. (Found)	%H Calc. (Found)	%N Calc. (Found)	%Metal Calc. (Found)
L	225-227 -	brown	746.4 (44.31)	6.12 (5.81)	20.40 (19.71)	-
[Cr LCl]Cl_2	>290	olive	54.27 (53.11)	5.15 (4.12)	13.96 (14.12)	10.36 (9.6)
[Zn LCl]Cl	300d	Cream	52.22 (51.00)	4.44 (4.88)	14.22 (14.66)	11.04 (10.84)
[Cd LCl]Cl	385d	yellow	47.88 (47.06)	4.02 (3.76)	13.30 (14.02)	21.34 (20.55)
[Hg LCl]Cl	366d	grey	40.58	3.41 (3.04)	11.27 (12.03)	33.34 (31.87)



Scheme (1) *synthesis of acyclic ligand N5*



M =Cr(III), x=2
M= Zn(II), Cd(II), Hg(II), X=1

Scheme (2) *synthesis of Metal complexes*

B-General procedure for preparation of complexes: The preparation of complexes was carried according to the method puplished in literature[8] (0.344gm, 0.01 mole) of N5 ligand in(10 ml) absolute ethanol was added drop wise with stirring to a solution of (0.01mole) of,($CdCl_2.4H_2O$,0.203gm) or anhydrous($ZnCl_2$,0.131gm, in 5ml methanol) or ($HgCl_2$, 0.271 gm) The reaction were carried out for 24-36 hrs and colored precipitate formed . These were filtered off washed with ethanol petroleum ether and dried on air. yields: 65% [Zn L Cl] Cl 60% [Cd L

Cl] Cl and 60% [Hg L Cl] Cl. The physical properties of metal chelate are shown in Scheme (2), Table (1).

C - preparation of Metal complexes: (0.26 g, 0.01 mol) of ($CrCl_3$. $6H_2O$) in (20 ml) methanol was added to(2g, 0.01mol) of ligand dissolved in methanolic potassium hydroxide to keep the pH of the solution for ≈8. The resulting mixture was refluxed under nitrogen atmosphere for 3 hrs until the green in solution became, then after cooling to room temperature green precipitate formed, filtered off, washed several times with 15ml of diethyl ether ,and dried under vacuum to offered (1.31 g, 65%) yield ,scheme(2).

3. Result and Discussion

3.1. IR and ^{13}CNMR Spectra

The IR spectra of the N4 ligand and its metal complexes provide information about the metal-ligand bonding. The medium doublet band in the region 3389-3325 cm^{-1} are assigned to $-NH_2$ group[9]. The strong absorption bands at 1637 cm^{-1} and 1589-1541 cm-1 are assigned to azomethine groups of C=N (terminal) and C=N of pyridine ring respectively[8] . These bands are shifted to lower wave number in the spectra of complexes (1620-1631cm^{-1}), which confirm the coordination of nitrogen atoms of C =N and nitrogen pyridine ring to metal ion via formation of six-membered ring , that is kinetically stable[3]. The change is intensity and sharp of a √NH_2 absorptions in the 3300-3400cm^{-1} revels participation of NH_2 group in coordination with metal ions understand therefore, the acyclic ligand behaviors pentadentate of N5- system. Weak absorption bands in the far red regions 400-600cm-1. The spectra of all metal complexes, provides good indication for M-N band[10, 11].

^{13}CNMR spectra of the ligand displayed signals corresponding to the various carbons of aromatic of phenyl and pyridine ring, as well as the de shielded absorptions of C=N in 120-135 region investigates the condensation of one mole of 2,6-diacetylpyridine with two moles of o-phenylenediamine to form acyclic ligand of N5type [12].Further support for formation of acyclic is the presence of absorptions in the downfield of ^{13}CNMR in figure 1 at 150-165 ppm assigning to carbon atoms of pyridine ring[12], this is good proof with conjugation of integrations of carbon atoms lay in the 20-25ppm region which reveals the two methyl groups in 2 and 6 positions of pyridine moiety[13].

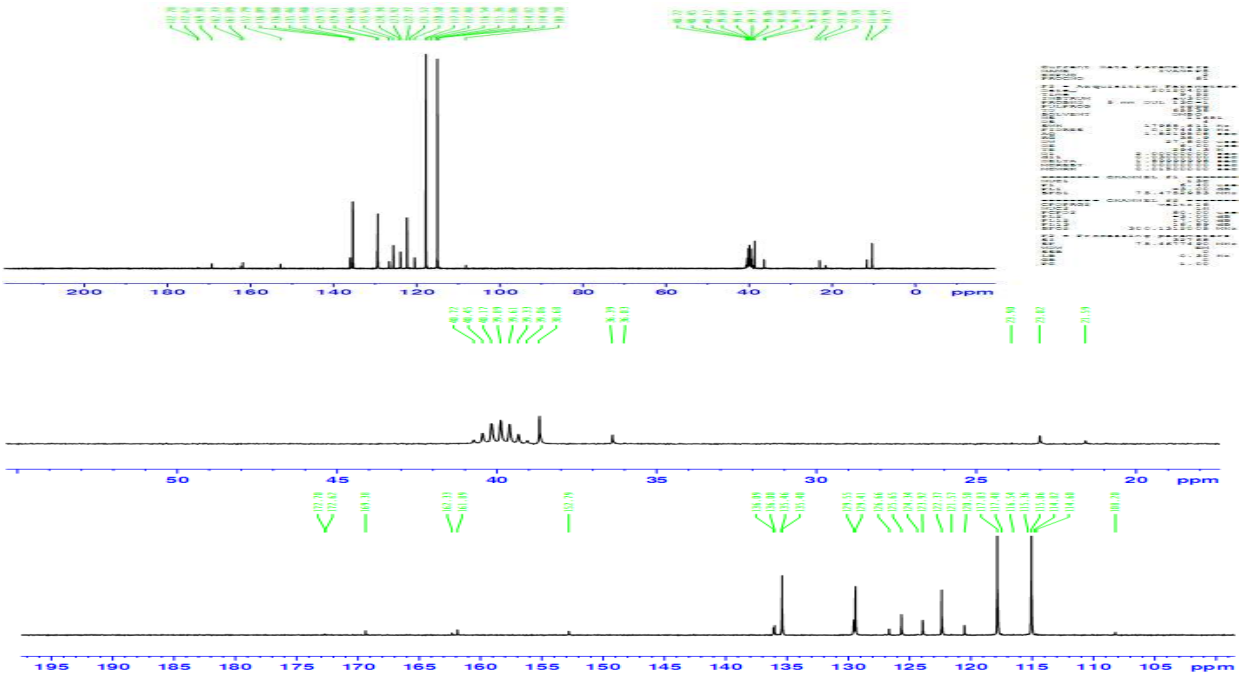


Figure (1) *^{13}C NMR spectrum of ligand in d6-DMSO.*

3.2. Electronic Spectra and Magnetic Properties

The electronic spectra of the ligand and metal complexes were recorded in absorbent ethanol and DMSO solution respectively , The ligand exhibits bands at 234 and 266nm, there are related to π→π* and n→π* transition of C=N, C=C chromophrous in the free ligand. The spectra of the complexes show bands in visible regions of spin-allowed transitions. The Cr(III) complex showed three d-d transitions at 625, 576 and 455nm which are assigned to $A_2g^4 \rightarrow T_2g^4$, T_1g^4 and $T_1g^4(p)$ respectively, Which reveals the octahedral environment around Cr(III) ion[13,14]. As well as the Zn(II), Cd(II) and Hg(II) complexes shows no d-d transition , but charge transfer in the 255nm region which investigation its octahedral geometry from elemental analysis .

The magnetic moments of divalent Cobalt, nickel, and

copper complexes lie in the 3.70, 2.25 and 1.30 B.M ranges respectively at room temperature and are close to the predicted value for octahedral geometry around the metal atom[15] .

3.3. Conductivity Measurement

The conductivity for 10^{-3}M solutions of metal complexes Table (3) in (DMSO) at 25 ^{o}C, show that Zn(II) , Cd(II) and Hg(II) to be 1:1 electrolyte. While Cr(III) complex shows electrolyte behavior in 1:2 ratio, this agrees well with the proposed formula of the complexes[16].

3.4. Atomic Absorption

The atomic absorption measurements Table(1) for all complexes gave approximated values for its theoretical.

Table (2) *IR spectra data of ligand of prepared compound*

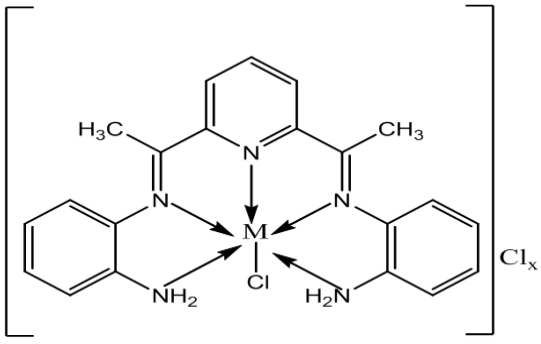
compound	υ (C=N)	υ (NH2)	υ (C-N) υ(C=N)(py)	υ (M-N)	υ (M-Cl)
L	1637(s)	3389-3365(m)	1589-1600	-	-
$[CrLCl]Cl_2$	1620	3340(br)	1554 (m)	500	390 (w)
[ZnLCl]Cl	1654	3400	1544 (m)	455(m)	377(w)
[CdLCl]Cl	1633	3245(br)	1533(s)	434(m)	319(w)
[HgLCl]Cl	1640(s)	3521(m)	1539(s)	421(w)	

W=weak, br=broad, s=strong, and m=medium

Table (3) *Electronic spectra ,magnetic moments and molar conductance of the prepared complexes*

Compound	λ max (nm)	assignment	M.eff (B.M)	ΔM (Ω^{-1} cm^2mol^{-1}) In DMSO
L	266	n→π*, π →π*		-
$[CrLCl]Cl_2$	287 625 576 455	L.F $^4A_2g(F)\rightarrow{}^4T_2g$ $^4A_2g(F) \rightarrow{}^4T_1g(F)$ $^4A_2g(F) \rightarrow{}^4T_1g(p)$	3.35	183
[ZnLCl]Cl	321, 360	n→π, LMCT	0	78
[CdLCl]Cl	255,370	π →π*,C.T	0	77
[HgLCl]Cl	218,347	π →π*,C.T	0	83

3.5. The Proposed Structure



M =Cr(III), x=2
M= Zn(II), Cd(II), Hg(II), X=1

Scheme (3) *The proposed structure of Metal complexes*

It is obviously, observed that free ligand of N5 system differs from N6-system, percent in literature[17-19]. where the reaction conditions of metal salts sported coordination with N4 system proceeds rapidly, rather than template system, this facts has investigation the basis of data obtained from ^{13}CNMR, FT-IR., UV-Vis., and others measurements.

A according to the elemental analysis, IR, UV-Vis. spectra and magnetic moment of complexes, all the complexes could have the proposed structure in Scheme (3) Where The ligand behavior pentadante of N5 system .

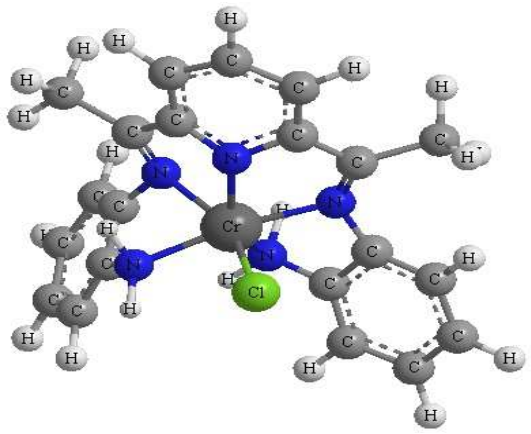


Fig (3) *The optimized structural geometry of Cr(III) complex*

Table (4) *structural parameters, bond length (ºA) and angles(º) of the [Cr(L)Cl]Cl complex*

Parameters	Parameters	Parameters
Bond angles(º)	Bond lengths (ºA)	Dihedral angles(º)
Cr(27)-Cl(28)2.1700	Cr(27)-Cl(28)2.1700	Cr(27)-Cl(28)2.1700
N(26)-H(47)1.0500	N(26)-H(47)1.0500	N(26)-H(47)1.0500
N(26)-Cr(27)1.8560	N(26)-Cr(27)1.8560	N(26)-Cr(27)1.8560
C(25)-H(46)1.1000	C(25)-H(46)1.1000	C(25)-H(46)1.1000
C(24)-C(25)1.3370	C(24)-C(25)1.3370	C(24)-C(25)1.3370
C(23)-N(26)1.9143	C(23)-N(26)1.9143	C(23)-N(26)1.9143
C(23)-C(24)1.3370	C(23)-C(24)1.3370	C(23)-C(24)1.3370
C(22)-H(45)1.1000	C(22)-H(45)1.1000	C(22)-H(45)1.1000
C(22)-C(23)1.3370	C(22)-C(23)1.3370	C(22)-C(23)1.3370
C(21)-H(44)1.1000	C(21)-H(44)1.1000	C(21)-H(44)1.1000
C(21)-C(22)1.3370	C(21)-C(22)1.3370	C(21)-C(22)1.3370
C(20)-H(43)1.1000	C(20)-H(43)1.1000	C(20)-H(43)1.1000
C(25)-C(20)1.3370	C(25)-C(20)1.3370	C(25)-C(20)1.3370
C(20)-C(21)1.3421	C(20)-C(21)1.3421	C(20)-C(21)1.3421
N(19)-H(42)1.0500	N(19)-H(42)1.0500	N(19)-H(42)1.0500
N(19)-Cr(27)1.8560	N(19)-Cr(27)1.8560	N(19)-Cr(27)1.8560
C(18)-H(41)1.1000	C(18)-H(41)1.1000	C(18)-H(41)1.1000
C(17)-H(40)1.1000	C(17)-H(40)1.1000	C(17)-H(40)1.1000
C(17)-C(18)1.3370	C(17)-C(18)1.3370	C(17)-C(18)1.3370
C(16)-H(39)1.1000	C(16)-H(39)1.1000	C(16)-H(39)1.1000
C(16)-C(17)1.3371	C(16)-C(17)1.3371	C(16)-C(17)1.3371
C(15)-H(38)1.1000	C(15)-H(38)1.1000	C(15)-H(38)1.1000
C(15)-C(16)1.3370	C(15)-C(16)1.3370	C(15)-C(16)1.3370
C(14)-N(19)1.3024	C(14)-N(19)1.3024	C(14)-N(19)1.3024
C(14)-C(15)1.3370	C(14)-C(15)1.3370	C(14)-C(15)1.3370
C(18)-C(13)1.3370	C(18)-C(13)1.3370	C(18)-C(13)1.3370
C(13)-C(14)1.3370	C(13)-C(14)1.3370	C(13)-C(14)1.3370
N(12)-Cr(27)1.8560	N(12)-Cr(27)1.8560	N(12)-Cr(27)1.8560
C(24)-N(12)1.2600	C(24)-N(12)1.2600	C(24)-N(12)1.2600
C(11)-H(37)1.1130	C(11)-H(37)1.1130	C(11)-H(37)1.1130
C(11)-H(36) 1130	C(11)-H(36)1.1130	C(11)-H(36)1.1130
C(11)-H(35)1.1130	C(11)-H(35)1.1130	C(11)-H(35)1.1130
C(10)-H(34)1.1130	C(10)-H(34)1.1130	C(10)-H(34)1.1130
C(10)-H(33)1.1130	C(10)-H(33)1.1130	C(10)-H(33)1.1130
C(10)-H(32)1.1130	C(10)-H(32)1.1130	C(10)-H(32)1.1130
C(9)-N(12)2.3547	C(9)-N(12)2.3547	C(9)-N(12)2.3547
C(9)-C(11)1.4970	C(9)-C(11)1.4970	C(9)-C(11)1.4970
N(8)-Cr(27)1.8560	N(8)-Cr(27)1.8560	N(8)-Cr(27)1.8560
C(13)-N(8)1.2600	C(13)-N(8)1.2600	C(13)-N(8)1.2600
C(7)-C(10)1.4970	C(7)-C(10)1.4970	C(7)-C(10)1.4970
C(7)-N(8) 2.2984	C(7)-N(8) 2.2984	C(7)-N(8) 2.2984
C(6)-H(31)1.1000	C(6)-H(31)1.1000	C(6)-H(31)1.1000
C(5)-H(30)1.1000	C(5)-H(30)1.1000	C(5)-H(30)1.1000
C(5)-C(6) 1.0286	C(5)-C(6)1.0286	C(5)-C(6)1.0286
C(4)-C(7) 1.3370	C(4)-C(7)1.3370	C(4)-C(7)1.3370
C(4)-C(5) 1.3370	C(4)-C(5)1.3370	C(4)-C(5)1.3370
N(3)-Cr(27)1.8560	N(3)-Cr(27)1.8560	N(3)-Cr(27)1.8560
N(3)-C(4) 1.2600	N(3)-C(4)1.2600	N(3)-C(4)1.2600
C(2)-C(9) 1.3370	C(2)-C(9)1.3370	C(2)-C(9)1.3370
C(2)-N(3) 1.2600	C(2)-N(3)1.2600	C(2)-N(3)1.2600
C(1)-H(29)1.1000	C(1)-H(29)1.1000	C(1)-H(29)1.1000
C(6)-C(1)1.3370	C(6)-C(1)1.3370	C(6)-C(1)1.3370
C(1)-C(2)1.3370	C(1)-C(2)1.3370	C(1)-C(2)1.3370
H(44)-C(21)-C(22)120.1266		H(44)-C(21)-C(22)120.1266
H(44)-C(21)-C(20)120.1267	Dihedral angles(º)	H(44)-C(21)-C(20)120.1267
C(22)-C(21)-C(20)119.7468	C(23)-N(26)-Cr(27)-N(3)134.2624	C(22)-C(21)-C(20)119.7468
H(43)-C(20)-C(25)120.1122	C(23)-N(26)-Cr(27)-N(8)44.2594	H(43)-C(20)-C(25)120.1122
H(43)-C(20)-C(21)120.1123	C(23)-N(26)-Cr(27)-N(12)44.2623	H(43)-C(20)-C(21)120.1123
C(25)-C(20)-C(21)119.7755	C(23)-N(26)-Cr(27)-N(19)44.2623	C(25)-C(20)-C(21)119.7755
H(46)-C(25)-C(24)119.9998	C(23)-N(26)-Cr(27)-Cl(28)-109.2857	H(46)-C(25)-C(24)119.9998
H(46)-C(25)-C(20)120.0006	H(47)-N(26)-Cr(27)-N(3)-45.7378	H(46)-C(25)-C(20)120.0006
C(24)-C(25)-C(20)119.9996	H(47)-N(26)-Cr(27)-N(8)-135.7408	C(24)-C(25)-C(20)119.9996
H(45)-C(22)-C(23)120.0000	H(47)-N(26)-Cr(27)-N(12)-135.7379	H(45)-C(22)-C(23)120.0000
H(45)-C(22)-C(21)120.0000	H(47)-N(26)-Cr(27)-N(19)-135.7379	H(45)-C(22)-C(21)120.0000
C(23)-C(22)-C(21)120.0000	H(47)-N(26)-Cr(27)-Cl(28)70.7141	C(23)-C(22)-C(21)120.0000

N(26)-C(23)-C(24)113.2601	N(12)-C(24)-C(25)-C(20)179.9999	N(26)-C(23)-C(24)113.2601
N(26)-C(23)-C(22)126.7382	N(12)-C(24)-C(25)-H(46)-0.0004	N(26)-C(23)-C(22)126.7382
C(24)-C(23)-C(22)119.9985	C(23)-C(24)-C(25)-C(20)0.7421	C(24)-C(23)-C(22)119.9985
H(40)-C(17)-C(18)120.0008	C(23)-C(24)-C(25)-H(46)-179.2583	H(40)-C(17)-C(18)120.0008
H(40)-C(17)-C(16)120.0008	C(22)-C(23)-N(26)-Cr(27)143.2547	H(40)-C(17)-C(16)120.0008
C(18)-C(17)-C(16)119.9985	C(22)-C(23)-N(26)-H(47)-36.7451	C(18)-C(17)-C(16)119.9985
H(39)-C(16)-C(17)120.0011	C(24)-C(23)-N(26)-Cr(27)-36.0883	H(39)-C(16)-C(17)120.0011
H(39)-C(16)-C(15)120.0009	C(24)-C(23)-N(26)-H(47)143.9119	H(39)-C(16)-C(15)120.0009
C(17)-C(16)-C(15)119.9980	C(22)-C(23)-C(24)-N(12)177.3357	C(17)-C(16)-C(15)119.9980
H(41)-C(18)-C(17)120.0002	C(22)-C(23)-C(24)-C(25)-3.2820	H(41)-C(18)-C(17)120.0002
H(41)-C(18)-C(13)119.9997	N(26)-C(23)-C(24)-N(12)-3.2722	H(41)-C(18)-C(13)119.9997
C(17)-C(18)-C(13)120.0001	N(26)-C(23)-C(24)-C(25)176.1100	C(17)-C(18)-C(13)120.0001
H(38)-C(15)-C(16)120.0001	C(21)-C(22)-C(23)-C(24)-0.0002	H(38)-C(15)-C(16)120.0001
H(38)-C(15)-C(14)120.0003	C(21)-C(22)-C(23)-N(26)-179.3032	H(38)-C(15)-C(14)120.0003
C(16)-C(15)-C(14)119.9996	H(45)-C(22)-C(23)-C(24)179.9998	C(16)-C(15)-C(14)119.9996
N(19)-C(14)-C(15)105.9067	H(45)-C(22)-C(23)-N(26)0.6968	N(19)-C(14)-C(15)105.9067
N(19)-C(14)-C(13)123.1518	C(20)-C(21)-C(22)-C(23)5.7928	N(19)-C(14)-C(13)123.1518
C(15)-C(14)-C(13)120.0007	C(20)-C(21)-C(22)-H(45)-174.2072	C(15)-C(14)-C(13)120.0007
H(47)-N(26)-Cr(27)138.4753	H(44)-C(21)-C(22)-C(23)-174.2070	H(47)-N(26)-Cr(27)138.4753
H(47)-N(26)-C(23)138.4755	H(44)-C(21)-C(22)-H(45)5.7930	H(47)-N(26)-C(23)138.4755
Cr(27)-N(26)-C(23)83.0492	C(24)-C(25)-C(20)-C(21)5.0530	Cr(27)-N(26)-C(23)83.0492
H(42)-N(19)-Cr(27)130.4344	C(24)-C(25)-C(20)-H(43)-174.9467	H(42)-N(19)-Cr(27)130.4344
H(42)-N(19)-C(14)130.4343	H(46)-C(25)-C(20)-C(21)-174.9466	H(42)-N(19)-C(14)130.4343
Cr(27)-N(19)-C(14)99.1313	H(46)-C(25)-C(20)-H(43)5.0537	Cr(27)-N(19)-C(14)99.1313
C(25)-C(24)-C(23)119.9987	C(25)-C(20)-C(21)-C(22)-8.3167	C(25)-C(24)-C(23)119.9987
C(25)-C(24)-N(12)128.9979	C(25)-C(20)-C(21)-H(44)171.6831	C(25)-C(24)-N(12)128.9979
C(23)-C(24)-N(12)110.9999	H(43)-C(20)-C(21)-C(22)171.6830	C(23)-C(24)-N(12)110.9999
H(37)-C(11)-H(36)109.5201	H(43)-C(20)-C(21)-H(44)-8.3172	H(37)-C(11)-H(36)109.5201
H(37)-C(11)-H(35)109.4612	C(14)-N(19)-Cr(27)-N(3)92.0068	H(37)-C(11)-H(35)109.4612
H(37)-C(11)-C(9)109.4617	C(14)-N(19)-Cr(27)-N(8)2.0070	H(37)-C(11)-C(9)109.4617
H(36)-C(11)-H(35)109.4423	C(14)-N(19)-Cr(27)-N(12)0.0000	H(36)-C(11)-H(35)109.4423
H(36)-C(11)-C(9)109.4419	C(14)-N(19)-Cr(27)-N(26)-177.9930	H(36)-C(11)-C(9)109.4419
H(35)-C(11)-C(9)109.5001	C(14)-N(19)-Cr(27)-Cl(28)-87.9956	H(35)-C(11)-C(9)109.5001
Cr(27)-N(12)-C(24)104.0001	H(42)-N(19)-Cr(27)-N(3)-87.9932	Cr(27)-N(12)-C(24)104.0001
Cr(27)-N(12)-C(9)82.6297	H(42)-N(19)-Cr(27)-N(8)-177.9931	Cr(27)-N(12)-C(9)82.6297
C(24)-N(12)-C(9)114.9998	H(42)-N(19)-Cr(27)-N(12)0.0000	C(24)-N(12)-C(9)114.9998
C(18)-C(13)-C(14)119.9980	H(42)-N(19)-Cr(27)-N(26)2.0069	C(18)-C(13)-C(14)119.9980
C(18)-C(13)-N(8)128.9979	H(42)-N(19)-Cr(27)-Cl(28)92.0043	C(18)-C(13)-N(8)128.9979
C(14)-C(13)-N(8)111.0006	C(16)-C(17)-C(18)-C(13)-0.2485	C(14)-C(13)-N(8)111.0006
H(34)-C(10)-H(33)109.5201	C(16)-C(17)-C(18)-H(41)179.7516	H(34)-C(10)-H(33)109.5201
H(34)-C(10)-H(32)109.4620	H(40)-C(17)-C(18)-C(13)179.7514	H(34)-C(10)-H(32)109.4620
H(34)-C(10)-C(7)109.4617	H(40)-C(17)-C(18)-H(41)-0.2485	H(34)-C(10)-C(7)109.4617
H(33)-C(10)-H(32)109.4419	C(15)-C(16)-C(17)-C(18)-0.3692	H(33)-C(10)-H(32)109.4419
H(33)-C(10)-C(7)109.4418	C(15)-C(16)-C(17)-H(40)179.6308	H(33)-C(10)-C(7)109.4418
H(32)-C(10)-C(7)109.4998	H(39)-C(16)-C(17)-C(18)179.6309	H(32)-C(10)-C(7)109.4998
Cr(27)-N(8)-C(13)103.9996	H(39)-C(16)-C(17)-H(40)-0.3690	Cr(27)-N(8)-C(13)103.9996
Cr(27)-N(8)-C(7)84.2196	C(14)-C(15)-C(16)-C(17)0.4936	Cr(27)-N(8)-C(7)84.2196
C(13)-N(8)-C(7)148.5254	C(14)-C(15)-C(16)-H(39)-179.5065	C(13)-N(8)-C(7)148.5254
H(31)-C(6)-C(5)122.1913	H(38)-C(15)-C(16)-C(17)-179.5066	H(31)-C(6)-C(5)122.1913
H(31)-C(6)-C(1)122.1911	H(38)-C(15)-C(16)-H(39)0.4932	H(31)-C(6)-C(1)122.1911
C(5)-C(6)-C(1)115.6176	C(13)-C(14)-N(19)-Cr(27)19.4981	C(5)-C(6)-C(1)115.6176
C(10)-C(7)-N(8)129.2349	C(13)-C(14)-N(19)-H(42)-160.5018	C(10)-C(7)-N(8)129.2349
C(10)-C(7)-C(4)129.2349	C(15)-C(14)-N(19)-Cr(27)163.3164	C(10)-C(7)-C(4)129.2349
N(8)-C(7)-C(4)101.5302	C(15)-C(14)-N(19)-H(42)-16.6835	N(8)-C(7)-C(4)101.5302
H(30)-C(5)-C(6)115.3091	C(13)-C(14)-C(15)-C(16)-0.0003	H(30)-C(5)-C(6)115.3091
H(30)-C(5)-C(4)115.3083	C(13)-C(14)-C(15)-H(38)180.0000	H(30)-C(5)-C(4)115.3083
C(6)-C(5)-C(4)129.3827	N(19)-C(14)-C(15)-C(16)-145.1999	C(6)-C(5)-C(4)129.3827
Cl(28)-Cr(27)-N(26)90.5117	N(19)-C(14)-C(15)-H(38)34.8004	Cl(28)-Cr(27)-N(26)90.5117
Cl(28)-Cr(27)-N(19)153.5492	C(17)-C(18)-C(13)-N(8)-180.0000	Cl(28)-Cr(27)-N(19)153.5492
Cl(28)-Cr(27)-N(12)153.5492	C(17)-C(18)-C(13)-C(14)0.7418	Cl(28)-Cr(27)-N(12)153.5492
Cl(28)-Cr(27)-N(8)90.0012	H(41)-C(18)-C(13)-N(8)-0.0001	Cl(28)-Cr(27)-N(8)90.0012
Cl(28)-Cr(27)-N(3)116.4507	H(41)-C(18)-C(13)-C(14)-179.2583	Cl(28)-Cr(27)-N(3)116.4507
N(26)-Cr(27)-N(19)89.4271	N(8)-C(13)-C(14)-C(15)-179.9999	N(26)-Cr(27)-N(19)89.4271
N(26)-Cr(27)-N(12)89.4271	N(8)-C(13)-C(14)-N(19)-40.9635	N(26)-Cr(27)-N(12)89.4271
N(26)-Cr(27)-N(8)179.4271	C(18)-C(13)-C(14)-C(15)-0.6175	N(26)-Cr(27)-N(8)179.4271
N(26)-Cr(27)-N(3)90.0001	C(18)-C(13)-C(14)-N(19)138.4190	N(26)-Cr(27)-N(3)90.0001
N(19)-Cr(27)-N(12)0.0000	C(9)-N(12)-Cr(27)-N(3)-39.0671	N(19)-Cr(27)-N(12)0.0000
N(19)-Cr(27)-N(8)90.0000	C(9)-N(12)-Cr(27)-N(8)-129.0670	N(19)-Cr(27)-N(8)90.0000

N(19)-Cr(27)-N(3)90.0001	C(9)-N(12)-Cr(27)-N(19)0.0000	N(19)-Cr(27)-N(3)90.0001
N(12)-Cr(27)-N(8)90.0000	C(9)-N(12)-Cr(27)-N(26)50.9330	N(12)-Cr(27)-N(8)90.0000
N(12)-Cr(27)-N(3)90.0001	C(9)-N(12)-Cr(27)-Cl(28)140.9304	N(12)-Cr(27)-N(3)90.0001
N(8)-Cr(27)-N(3)89.9999	C(24)-N(12)-Cr(27)-N(3)-153.0793	N(8)-Cr(27)-N(3)89.9999
C(7)-C(4)-C(5)128.9989	C(24)-N(12)-Cr(27)-N(8)116.9208	C(7)-C(4)-C(5)128.9989
C(7)-C(4)-N(3)110.9986	C(24)-N(12)-Cr(27)-N(19)0.0000	C(7)-C(4)-N(3)110.9986
C(5)-C(4)-N(3)119.9999	C(24)-N(12)-Cr(27)-N(26)-63.0792	C(5)-C(4)-N(3)119.9999

3.6. Theoretical Study

The ball and cylinders and some of selected structural parameters (bond lengthand angles) of the optimized geometries are shown in table (4) fig. (3). As shown in this figure, there is no obvious trend for the variation of these parameters. The values of the bond length and angles of the optimized geometries are quite similar to the experimental results of the corresponding compounds.

4. Conclusions

From the analytical and spectral data, it is concluded that the present ligand, L, act as potential pentadentate systems. Physical and spectroscopic characterization of all the prepared complexes had octahedral geometry.

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