THEORETICAL STUDY OF THE CHARACTERIZATION OF MIXED-LIGAND COMPLEXES OF Ni (II) DIMETHYLGLYOXIME

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(Received: 19th May, 2015; Accepted: 14th July, 2015)

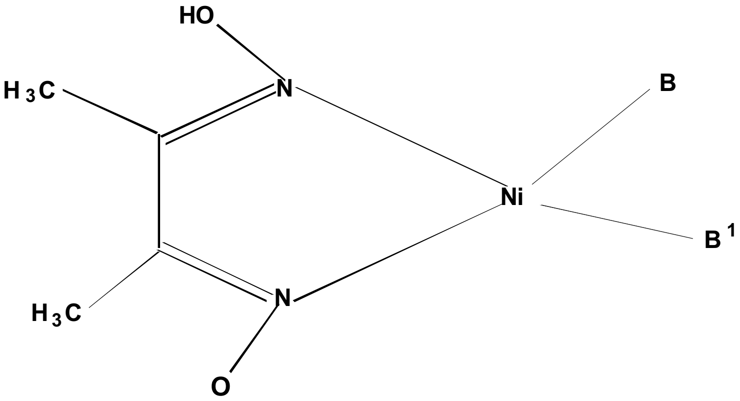
ABSTRACT

The non-electrolyte mixed-ligand complexes of the general formula [M(Hdmg)B], M=Ni(II), Hdmg=dimethylgloximato monoanion, B=2-aminophenol (2-aph), diethylamine (dea) or malonic acid (MOH) were synthesized and characterized. However theoretical calculations were carried out to obtained the geometric and thermodynamic parameters, vibrational and electronic properties, dipole moments and HOMO-LUMO band gaps of the complex with different substituents. These properties were obtained using the PM3 and DFT with B3LYP at 6-31G* level. Comparisons were made on the calculated bond length, bond angle, dihedrals and vibrational frequencies and it was observed that the calculated data were in good agreement with experimental data.

Keywords: Geometric Parameters, Dipole Moments, Band Gaps Modelling.

INTRODUCTION

The term computational chemistry is generally used when a mathematical method is sufficiently well developed that it can be used automatically on a computer. Quantum mechanics gives a mathematical description of the behavior of electrons that have never been found to be wrong. However, the quantum mechanical equations have never been solved exactly for any chemical system other than the hydrogen atom. Thus, the entire field of computational chemistry is built around approximate solutions. Some of these solutions are very crude but are still more accurate than any experiment that has yet been conducted (David, 2001). It also helps chemists to make predictions before running the actual experiment so that they can be better prepared for making observations (Shodor, 2000). Chelation chemistry has been gaining recognition in recent times because of its great importance in medicine and related areas of life sciences. It is also important in the design of respiratory, slow and controlled release of drugs. It has also been established that the efficacies of some therapeutic agents increase upon coordination (Ajibola, 1990; Obaleye *et al.*, 1997). Metal complexes, especially mixed-ligands are reported to exhibit different activities (Kudirat *et al.*, 1994; Yeamin *et al.*, 2003; Oguniran *et al.*, 2007). Molecular modeling is an aspect of computational chemistry that gives accurate results compared with experimental results. It is used to account for properties such as bond length, bond angle, dihedrals vibrational frequencies, atomic charge distributions etc (Conradie, 2010). PM3 semi empirical quantum mechanical calculations were carried out on a Novel Dichlorobis (N-{4-[(2-pyrimidinyl-kNamino)sulfonyl} acetamide]copper(II), containing a metabolite N-acetylsulfadiazine and the result obtained compared perfectly well with the experimental data. (Adejoro *et al.*, 2012). Calculations on novel polymeric Zn (II) complex containing the anti-malarial Quinine as ligands gave values that agreed perfectly well with experimental data (Adejoro *et al.*, 2013). Theoretical calculations on novel aminopyridino – 1-4-η-cyclohexa-1, 3-diene iron tricarbonyl complexes revealed that the complex was thermodynamically stable (Odiaka *et al.,* 2010). Theoretical calculations were done on mixed-ligand complexes (Scheme 1) of Co(II) dimethylglyoxime (Adejoro *et al.,* 2014a) and Cu(II) dimethylglyoxime (Adejoro *et al.,* 2014b). This work used theoretical approach using semi-empirical PM3 and Density Functional Theory (DFT) methods of calculation in Spartan to validate the experimental result obtained by Osunlaja *et al.*, 2011.



Scheme 1: Structure of the complex B= 2-aminophenol(2-aph) B^1 = Hydrogen
B= diethylamine (dea) B^1 = diethylamine(dea)
B= malonic acid (MOH) B^1 = Hydrogen

COMPUTATIONAL METHODOLOGY

Conformational search was performed on the molecule to locate the structure with the lowest energy. The conformational search were carried out using molecular mechanics force field (MMFF) which is quite successful in assigning low energy conformers and in providing quantitative estimates of conformational energy differences (Warren, 2003). Semi-empirical PM3 and Density functional methods were used to carry out molecular calculations on the complexes. The structures were fully optimized (Figs. 1a, b and c) and geometric calculations were done to obtain the bond length, bond angle, and bond dihedrals of the complexes. Thermodynamic calculations, vibrational and electronic properties, heat of formation, dipole moment, E-HOMO, E-LUMO and band gaps were calculated.

Calculations

Thermodynamic, band gaps and electronic calculations were done using the equations below:

$$\Delta G = \Delta H - T\Delta S \qquad (1)$$

Where ΔG is the free energy change of formation.

ΔH is the enthalpy change of formation

ΔS is the entropy change

T is temperature at 298 kelvin

The band gap and electronic properties were calculated using:

$$E_{gap} = E_{Lumo} - E_{Homo} \qquad (2)$$

where E_{gap} is the energy gap

E_{Lumo} is the energy of the lowest unoccupied molecular orbital

E_{Homo} is the energy of the highest occupied molecular orbital

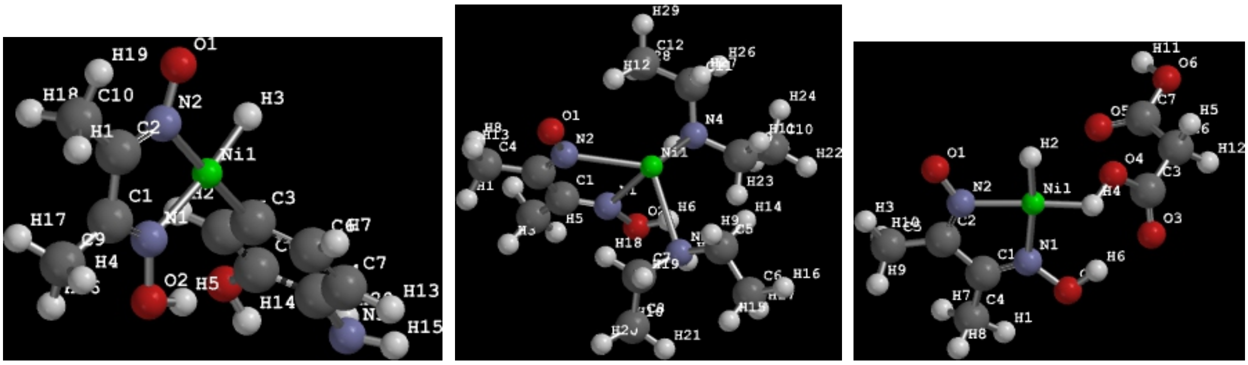


Fig1a: NiHdmg(2-aph) **Fig 1b**:NiHdmg(dea)$_2$ **Fig 1c:** NiHdmg(MO)

Fig. 1: The Structures of Mixed-ligand of Ni (II), Complex.

RESULTS AND DISCUSSION

Geometric Parameters:

Calculations were carried out on the structure with the lowest values; this was obtained using confomer distribution calculation with MMFF$_{aq.}$ Geometric parameters were obtained after optimization using PM3, DFT (6-31G*). The bond distances, bond angles, and dihedrals are shown Tables 1- 3.

Table 1: Selected Bond Distances, Bond Angles, and Dihedrals of 2- aminophenol Dimethylglyoxime Nickel(II) (Å)

Bond length	**PM3**	**DFT/ B3LYP 6-31G**	**Bond angles**	**PM3**	**DFT/ B3LYP 6-31G**	**Dihedrals**	**PM3**	**DFT/ B3LYP 6-31G***
Ni_1-H_2	1.7794	2.8825	$Ni_1-N_3-C_5$	106.294	115.257	$Ni_1-N_4-C_6-C_5$	-0.220	1.632
Ni_1-N_3	1.8217	1.8635	$Ni_1-N_3-O_8$	79.774	125.071	$Ni_1-N_3-C_5-C_6$	18.538	6.756
Ni_1-N_4	1.7881	1.8517	$Ni_1-N_4-C_6$	109.706	115.328	$Ni_1-C_{10}-C_{12}-C_{15}$	-160.345	-55.201
Ni_1-C_{10}	2.1865	2.1516	$Ni_1-N_4-O_7$	119.615	120.319	$Ni_1-C_{10}-C_{13}-C_{14}$	120.022	56.072
N_3-C_5	1.4358	1.3140	$Ni_1-C_{10}-C_{12}$	69.587	75.286	$Ni_1-N_3-O_{18}-H_9$	-161.599	-48.693
N_3-O_8	1.4847	1.3893	$Ni_1-C_{10}-C_{13}$	161.834	72.350	$Ni_1-C_{10}-C_{12}-H_{16}$	32.318	122.086
N_4-C_6	1.4243	1.3359	$H_2-Ni_1-N_3$	173.553	165.006	$Ni_1-N_4-C_6-C_{23}$	177.360	-178.023
N_4-O_7	1.1832	1.2467	$H_2-Ni_1-N_4$	90.477	81.632	$H_2-Ni_1-N_3-C_5$	92.568	-5.402
C_5-C_6	1.3734	1.4396	$H_2-Ni_1-C_{10}$	33.826	18.490	$H_2-Ni_1-N_4-C_6$	-164.705	-178.649
C_5-C_{19}	1.4695	1.4952	$N_3-Ni_1-H_2$	173.553	165.006	$H_2-Ni_1-N_4-O_7$	12.078	1.521

Table2: Selected Bond Distances, Bond Angles, And Dihedrals of Diethylamine Dimethylglyoxime Nickel(II) (Å)

Bond length	**PM3**	**DFT/ B3LYP 6-31G**	**bond angles**	**PM3**	**DFT/ B3LYP 6-31G**	**Dihedrals**	**PM3**	**DFT/ B3LYP 6-31G**
Ni_1-N_2	1.8470	1.8802	$Ni_1-N_2-C_8$	108.362	116.230	$Ni_1-N_3-C_9-C_8$	-6.073	1.682
Ni_1-N_3	1.7981	1.8963	$Ni_1-N_2-O_{11}$	81.974	124.684	$Ni_1-N_2-C_8-C_9$	-11.874	-9.834
Ni_1-N_4	1.9228	1.9535	$Ni_1-N_3-C_9$	111.574	115.492	$Ni_1-N_2-O_{11}-H_2$	171.558	110.618
Ni_1-N_6	1.9391	1.9751	$Ni_1-N_3-O_{10}$	121.267	124.829	$Ni_1-N_2-C_8-C_{13}$	170.499	171.770
N_2-C_8	1.4308	1.3211	$Ni_1-N_4-H_5$	108.151	106.965	$Ni_1-N_3-C_9-C_{17}$	176.404	-178.870
N_2-O_{11}	1.5042	1.4160	$Ni_1-N_4-C_{21}$	96.817	111.681	$Ni_1-N_4-C_{21}-H_{22}$	111.919	62.220
N_3-C_9	1.4280	1.3421	$Ni_1-N_4-C_{28}$	131.790	111.706	$Ni_1-N_4-C_{21}-H_{23}$	-4.204	-52.642
N_3-O_{10}	1.1908	1.2576	$Ni_1-N_6-H_7$	110.477	100.387	$Ni_1-N_4-C_{21}-C_{24}$	-125.898	-174.299
N_4-H_5	1.0018	1.0210	$Ni_1-N_6-C_{35}$	89.824	112.829	$Ni_1-N_4-C_{28}-H_{29}$	-52.992	13.290

Table 3: Selected Bond Distances, Bond Angles and Dihedrals for the Malonic Acid Dimethylglyoxime Nickel(II) (Å)

Bond Length	PM3	**DFT/ B3LYP 6-31G**	**bond angles**	PM3	**DFT/ B3LYP 6-31G**	**Dihedrals**	PM3	**DFT/ B3LYP 6-31G**
Ni_1-H_2	1.6055	1.4804	$Ni_1-N_3-C_5$	97.966	111.805	$Ni_1-N_4-C_6-C_5$	-9.563	-4.873
Ni_1-N_3	1.8741	1.9014	$Ni_1-N_3-O_8$	91.614	121.745	$Ni_1-N_3-C_5-C_6$	40.765	20.966
Ni_1-N_4	1.7816	1.8270	$Ni_1-N_4-C_6$	105.348	113.670	$Ni_1-N_3-O_8-H_9$	-157.951	-110.168
Ni_1-H_{10}	2.4220	2.4282	$Ni_1-N_4-O_7$	127.557	127.436	$Ni_1-H_{10}-O_{13}-C_{11}$	-123.165	-154.043
N_3-C_5	1.4017	1.3273	$Ni_1-H_{10}-O_{13}$	47.481	50.031	$Ni_1-N_3-C_5-C_{14}$	-142.129	-162.018
N_3-O_8	1.4541	1.4413	$H_2-Ni_1-N_3$	175.752	170.807	$Ni_1-N_4-C_6-C_{18}$	167.788	179.026
N_4-C_6	1.4192	1.3640	$H_2-Ni_1-N_4$	88.805	92.573	$H_2-Ni_1-N_3-C_5$	40.366	48.250
N_4-O_7	1.1930	1.2493	$H_2-Ni_1-H_{10}$	103.141	117.377	$H_2-Ni_1-N_4-C_6$	-148.000	-158.575
C_5-C_6	1.3966	1.4198	$N_3-Ni_1-H_2$	175.752	170.807	$H_2-Ni_1-N_4-C_7$	32.769	21.822
C_5-C_{14}	1.4773	1.4413	$N_3-Ni_1-N_4$	90.339	83.843	$H_2-Ni_1-N_3-O_8$	-74.306	-95.583

Electronic Properties:

The electronic structure of the metal complex is described by its band structure (David, 2001). This is obtained from HOMO-LUMO calculation. The calculated HOMO-LUMO band gap using PM3 method is greater than that of the DFT/B3LYP/6-31G*. PM3 calculation for NiHdmg(2-aph) is +6.64, NiHdmg(dea)$_2$ is +8.06 and NiHdmg(MO) is +8.06 while with DFT/B3LYP/6-31G* it is +3.01, 7.13 and 3.55eV for the three complexes repectively (Table 4). This result shows that PM3 method have a better predictive ability on the stability of the metal complexes compared with DFT/B3LYP/6-31G* method.

Table 4: Electronic Properties of the Ni (II) complexes

COMPLEXES	Dipole moment/debye		EHOMO/ eV		ELUMO/eV		Bandgap/Ev	
	PM3	DFT	PM3	DFT	PM3	DFT	PM3	DFT
NiHdmg(2-aph)	1.54	5.69	-12.08	-9.23	-5.44	-6.64	+6.64	+3.01
NiHdmg (dea)$_2$	1.55	4.46	-8.94	-8.87	-0.88	-1.74	+8.06	+7.13
NiHdmg(MO)	3.75	3.59	-8.94	5.29	-0.88	-1.74	+8.06	+3.55

Thermodynamic Properties and Stabilities

The stability of a complex depends greatly on the thermodynamic parameters. Complexes are thermodynamically stable if ΔG and ΔH are negative. The more negative ΔG and ΔH, the more positive ΔS and the more stable the complex becomes. As shown in Table 5 with Pm3 ΔG (-0.218, -0.226 and -0.778), ΔH (-0.161, -0.161 and -0.722) and ΔS (499.03, 491.75 and 491.73), with DFT/B3LYP/6-31G* ΔG (-2287.091, -2351.755 and -2342.723), ΔH (-2287.034, -2351.686 and -2342.666) and ΔS (505.82, 504.68 and 504.68) for NiHdmg(2-aph), NiHdmg(dea)$_2$ and NiHdmg(MO) respectively. The values as obtained from DFT at B3LYP level with 6-31G* basis set, predicts the stability of the Dimethylglyoxime Ni(II) complexes better compared with PM3.

Table 5 : Thermodynamic Properties of the Nickel(II) complexes

COMPLEXES	Methods	Heat of formation $kJmol^{-1}$	SCF Total energy/au	Free energy/ au	Enthalpy/ au	Entropy $Jmol^{-1}K^{-1}$
NiHdmg(2aph)	PM3	-1104.503	-	-0.218	-0.161	499.03
	DFT/6-31G*	-	-2287.293	-2287.091	-2287.034	505.82
NiHdmg(dea)$_2$	PM3	-1583.084	-	-0.226	-0.161	491.75
	DFT/6-31G*	-	-2352.134	-2351.755	-2351.686	504.68
NiHdmg(MO)	PM3	-2495.829	-	-0.778	-0.722	491.73
	DFT/6-31G*	-	-2342.723	-2342.723	-2342.66	504.68

Vibrational Frequencies

The vibrational frequencies obtained theoretically were in perfect agreement with experimental result and experimental spectral results suggest the binding of Hdmg, 2-amino phenol or malonic acid through the N atom and O atoms respectively to the metal ion. It was discovered that DFT with basis set 6-31G* has values closer to experimental values. The absorption bands and their corresponding vibrations for the three complxes are shown Tables 6 with their corresponding IR spectra in Figures 2a, b and c. The υ(O-H) obtained with DFT(3717–3547 cm^{-1}), (3658 cm^{-1}) and (3682–3687 cm^{-1}) for 2-aph, $(dea)_2$ and MO respectively compared well with experimental values which are attributed to the O---H-O hydrogen bridges between the dimethylglyoximato ions (Nakamoto, 1986). The band υ(N-H) (3578–3489 cm^{-1}) and (3456-3392 cm^{-1}), υ(N-O) (1378 cm^{-1}), (1521-1509 cm^{-1}) and (1519 cm^{-1}) are also closer to experimental values while there is a large variation between the theoretical band obtained for υ(Ni-N) (3120 – 3066, 866 and 1037 cm^{-1}) compared with experimental data (520 cm^{-1}) for 2-aph, $(dea)_2$ and MO respectively.

Table 6: Absorption Bands with their Corresponding Vibration. Ni (II) Complexes (cm^{-1})

Complexes	Vibrations	Experimental	PM3	DFT
NiHdmg (2aph)	O–H stretching	3415	3862 – 3827	3717 – 3547
	N-H stretching	3253	3528 – 3411	3578 – 3489
	Ni-N stretching	520	1161	3120 – 3066
	N-O stretching	1240	2006	1378
	Ni–H stretching	N/A	2288	3259
	C–C stretching	N/A	1769	1529
	C–N stretching	N/A	1492	1636 – 1558
	C=C stretching	N/A	1082	1623
	C-H saturation	N/A	3157-3144	1558
	C-H aromatic	N/A	3065 – 3025	3247 – 3220
NiHdmg $(dea)_2$	O – Hstretching	3446	3819	3658
	C = Nstretching	1462	1502	1588
	Ni – Nstretching	520	792	866
	N – Ostretching	1239	1960	1521-1509
	N – Hstretching	N/A	3339-3317	3456-3392
	C – Hstretching	N/A	3182-3178	3185
	C – Cstretching	N/A	1791	1541
	C – Hbending	N/A	1447	1072
Ni Hdmg (MO)	O–H stretching	3443	3872-3623	3682 – 3687
	C-O stretching	1377	1983	1889-1828
	N-O saturation	1239	1966 – 1958	1519
	Ni-N stretching	520	1136	1037
	C-N stretching	1461	1559 -1370	1567 – 1334
	Cu-H stretching	N/A	3664 – 3129	3653 – 2009
	C–C stretching	N/A	1708 – 1319	1547
	C–H stretching	N/A	3012 – 2954	3148 – 3094
	Ni–H stretching	N/A	1183	1911
	C-H saturation	N/A	3161-3129	3653

NB: Experimental data (Nikamoto, 1996)

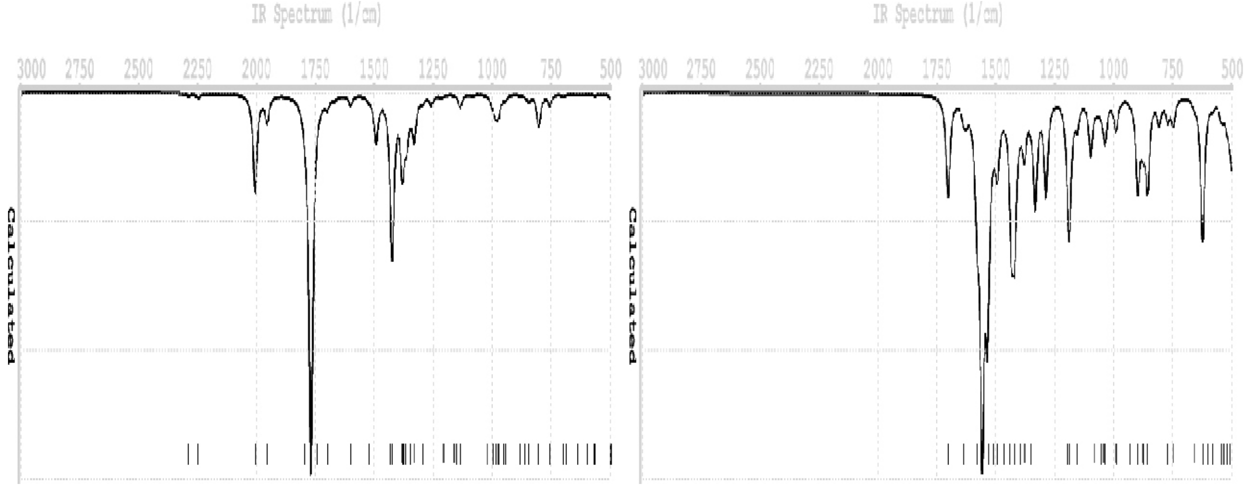


Fig 2a NiHdmg(2-aph) with PM3 with DFT/B3LYP/6-31G*

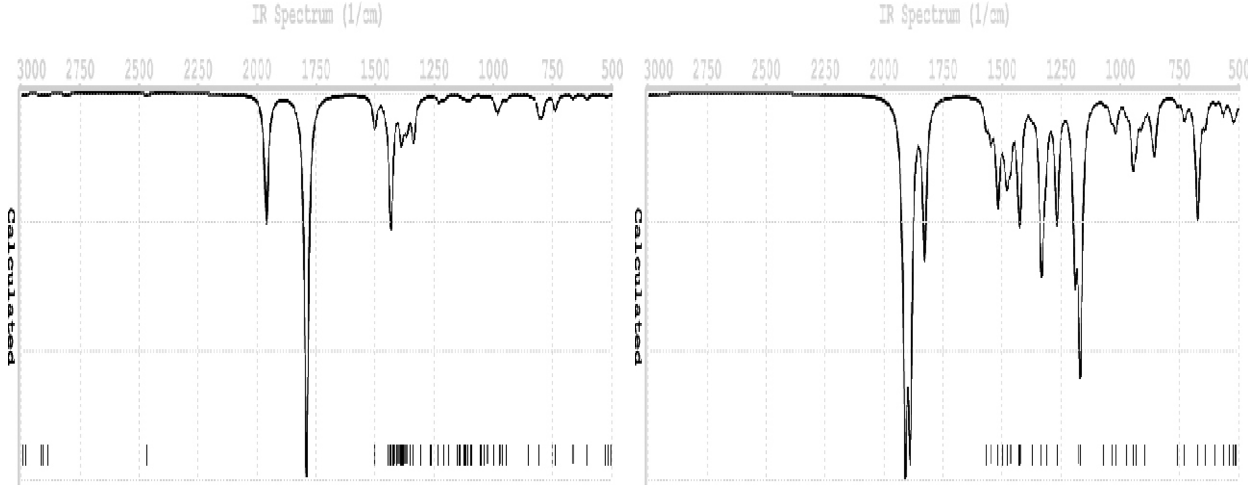


Fig. 2b: NiHdmg(dea)$_2$ with PM3 with DFT/B3LYP/6-31G*

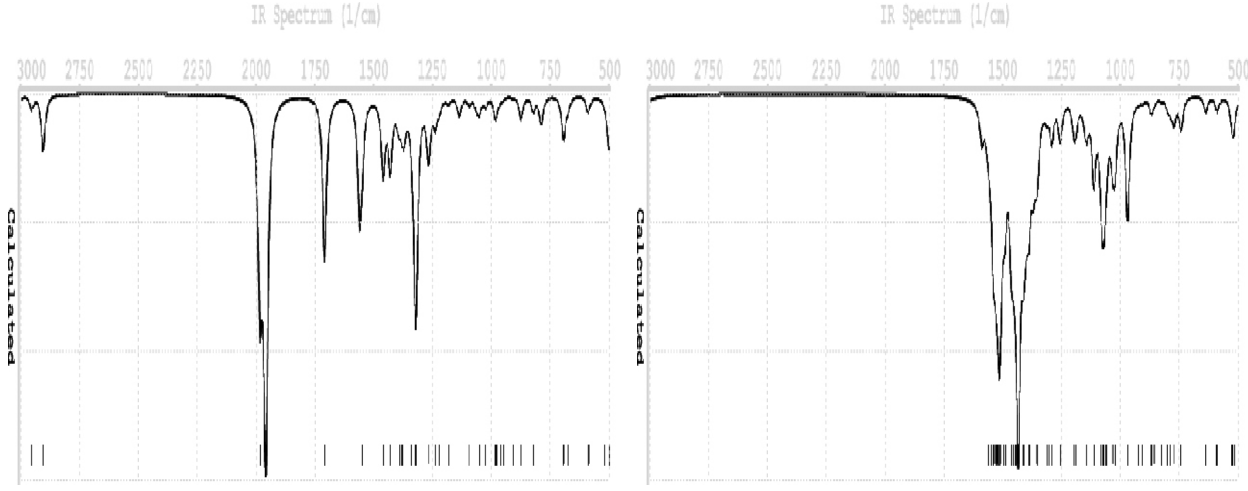


Fig. 2c: NiHdmg(MO) with PM3 with DFT/B3LYP/6-31G*

Electronic Spectra

In the electronic spectra of the complexes, the absorption bands observed in the UV/Visible region (Table 7) are presumed to be either due to charge transfer or intra-ligand transitions from the ligands or d-d transitions from the metal ions. The UV/Visible spectra data except for [Ni(Hdmg)(MO)] showed two major absorption bands as reported experimentally and the two d-d transition are assigned to $^3T_{1g}(F) \rightarrow {}^3A_{2g}$ and $^3T_{2g}(F) \rightarrow {}^3A_{2g}$ respectively (Osunlaja *et al.,* 2011). The UV/Visible spectrum of NiHdmg(2-aph) (Fig. 3a) showed well resolved absorption bands at 398 nm and 343 nm. These transitions are attributed to metal-ligand charge transfer transitions while the band at 456 nm may account for d-d transition with d-orbital of the metal ion. The UV/Visible spectrum of NiHdmg(dea), (Fig. 3b) presents two distinct bands at 383 nm and 427 nm attributed to metal-ligand charge transition while the unresolved band at 452 nm may account for d-d transition with d-orbital of the metal ion. Likewise the bands in the UV/Visible spectrum of NiHdgm(MO) (Fig. 3c) at 425 nm, 440 nm and 476 nm are due to metal-ligand charge transfer transitions while the band at 511 nm is attributed to the d-d transition within the d-orbitals of the metal ion.

Table 7: Absorption Bands (UV/Visible) with their Corresponding Intensiites (nm)

NiHdmg (2-aph)		NiHdmg (dea)$_2$		NiHdmg (MO)	
Wavelength	Intensity	Wavelength	Intensity	Wavelength	Intensity
398.48	0.0252079	383.96	0.0112627	425.21	0.00103689
343.65	0.0107276	427.19	0.00376201	440.97	0.00366562
456.93	0.00341757	452.32	0.00155451	476.55	0.00230483
539.63	0.00751611	473.91	0.000143928	511.68	0.00202609
674.35	0.000340581	527.78	0.001181173	564.12	0.00280195
742.59	0.00161888	549.05	0.00123535	577.02	0.00282956

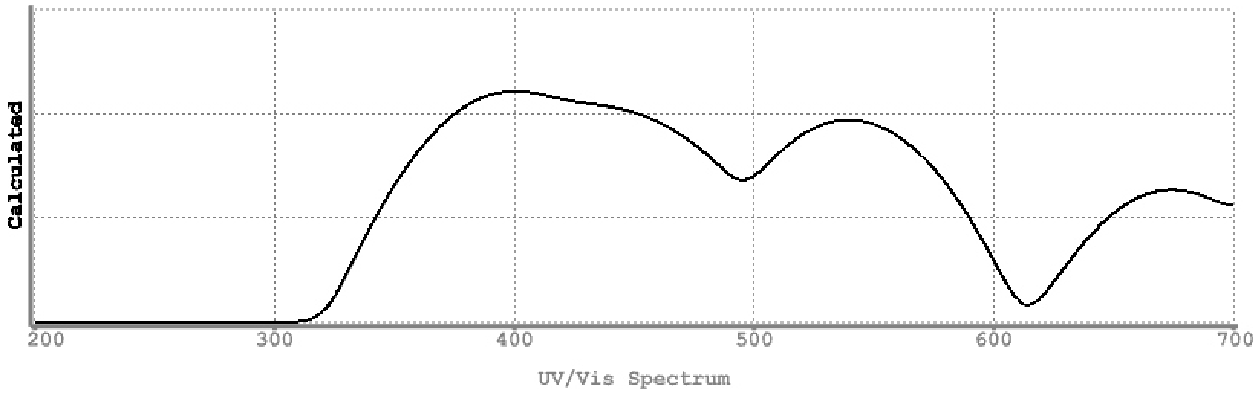


Fig 3aUltra-Violet/Visible Spectra of AminophenolDimethylglyoxime Nickel(II)

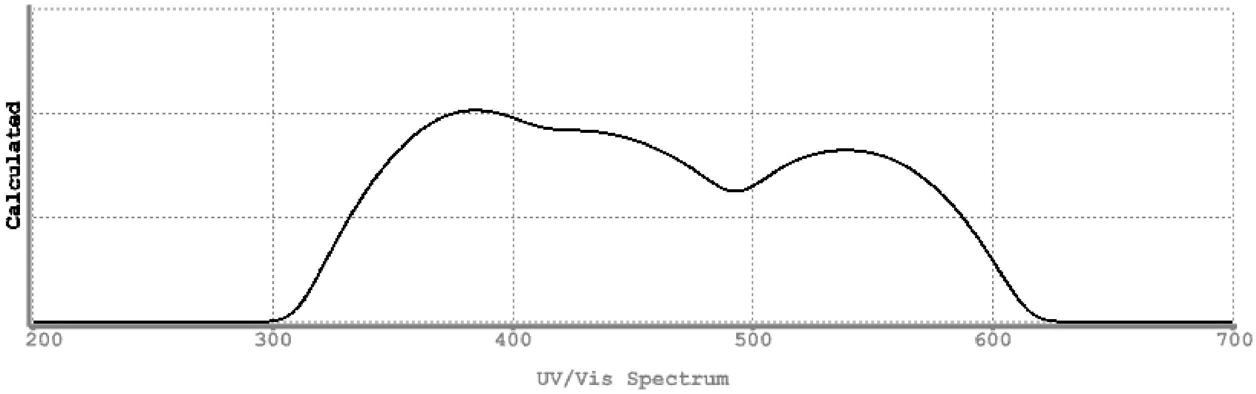


Fig 3b: Ultra-Violet/Visible Spectra of Diethylamine Dimethylglyoxime Nickel(II)

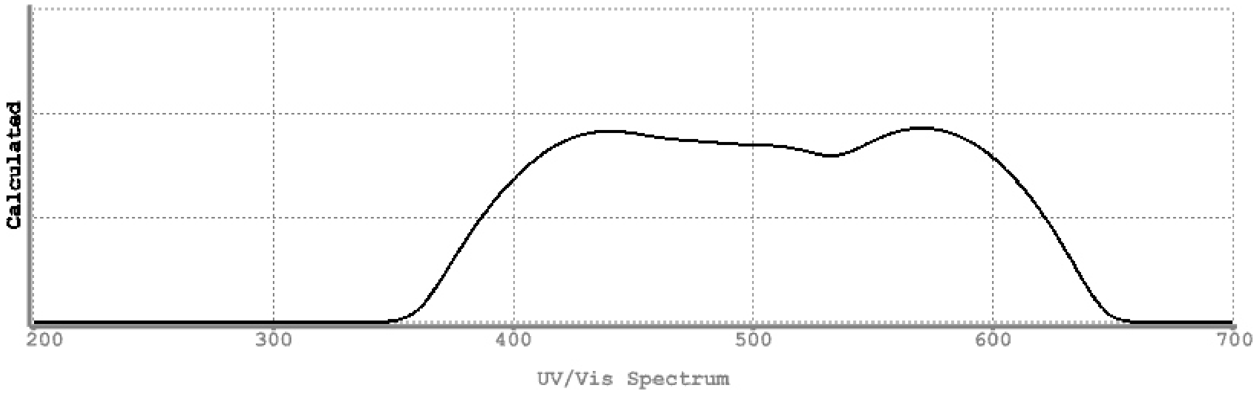


Fig 3c: Ultra-Violet/Visible Spectra of Malonic acid Dimethylglyoxime Nickel(II)

CONCLUSION

The properties of the Ni(II) mixed-ligand complexes of dimethylglyoxime were calculated using Semi-empirical and DFT methods. The optimized geometries, dipole moments, geometric, thermodynamics, vibrational and electronic parameters were investigated. Computational method has presented us the opportunity to take a critical look at this mixed-ligand complexes of dimethylglyoxime to produce results which compared favourably well with experimental data. It has also given us the opportunity to compute results on the properties that cannot be obtained in laboratory experiments. In studying and predicting the geometric parameters, vibrational and electronic properties of these compounds, the PM3 semi-empirical method accounted well for the geometric parameters while the DFT/B3LYP/6-31G*, for the vibrational and electronic frequencies. It can then be concluded that both methods (Semi-empirical PM3 and DFT/B3LYP) could be used for predicting the properties of transition metal complexes.

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