



Trends in Molecular Sciences

ISSN 1994-5469

science
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Quantum Mechanical Characterization of Mixed-Ligand Complex of Co(II) Dimethylglyoxime

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ABSTRACT

Non-electrolyte mixed-ligand complex of the general formula [Co(Hdmg)B], where Hdmg = dimethylglyoximate monoanion, B = 2-aminophenol(2-aph), diethylamine (dea) or malonic acid (MOH) has been synthesized and characterized. The aim of this study is to use quantum mechanical approach to elucidate the geometries and thermodynamic parameters, vibrational frequencies, dipole moments and HOMO-LUMO band gaps of the complex with different substituents were carried out. These properties were obtained using the PM3 and DFT with B3LYP at 6-31G* level. The uv/visible spectrum of CoHdmg(dea)₂ showed well resolved absorption bands at 467, 485 nm, these transitions are attributed to metal-ligand charge transfer transitions while the band at 535 nm is assigned to d-d transition within the metal. The uv/visible spectrum of CoHdmg(2aph) presents three distinct bands at 497, 650 nm attributed to metal-ligand charge transition while the band at 650 nm may account for d-d transition with d-orbital of the metal ion. Likewise the three prominent bands in the uv/visible spectrum of CoHdmg(MO) at 451, 463 nm are metal-ligand charge transfer transitions while the band at 570 nm is attributed to the d-d transition within the d-orbitals of the metal ion. It was observed that the calculated data are in good agreement with experimental data.

Key words: Geometric parameters, dipole moments, band gaps, modelling

INTRODUCTION

Metal complexes are of great importance in drug design and related areas of life sciences (Bulman, 1994). Efficacies of some therapeutic agents are known to increase upon coordination (Obaleye *et al.*, 2007). Mixed-ligand complexes are of great importance, they are known to exhibit remarkable activities (Kudirat *et al.*, 1994; Reza *et al.*, 2003; Ogunniran *et al.*, 2007; Shaker *et al.*, 2009). Computational chemistry is a method that is used to investigate materials that are too expensive to buy. It also helps chemists to make predictions before running the actual experiment so that they can be better prepared for making observations (Barden and Schaeffer, 2000). 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). Semi-empirical calculations were carried out on orotic acid mixed with zinc (II) dehydrate acetate in a neutral medium and it was observed that the calculated results agree well with experimental results (Gloria *et al.*, 2005). Theoretical calculations on novel aminopyridino -1-4-η-cyclohexa-1, 3-diene

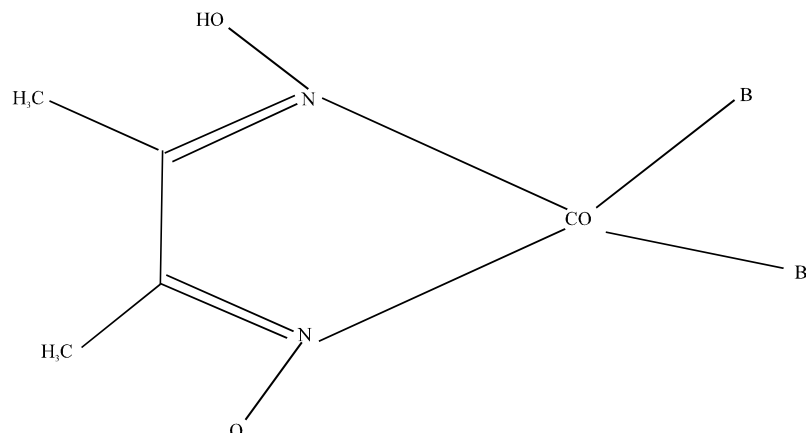


Fig. 1: Structure of the complex B= 2-aminophenol(2-aph) B¹ = Hydrogen, B = Diethylamine (dea) B¹ = Diethylamine(dea), B = Malonic acid (MOH) B¹ = Hydrogen

iron tricarbonyl complexes reveals that the complex is thermodynamically stable (Odiaka *et al.*, 2012). Calculations on novel polymeric Zn (II) complex containing the anti-malarial Quinine as ligands gives values that agrees perfectly well with experimental data (Adejoro *et al.*, 2013).

This article studied the quantum mechanical calculation on the experimental results that were carried out on the molecule (Osunlaja *et al.*, 2011). The complex were modelled using Spartan'10 and calculations were carried out on the optimized geometries of the most stable structure (Fig. 1).

MATERIALS AND METHODS

Computational methodology: Conformational search was performed on the molecule to locate the structure with the lowest energy. The conformational search was 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 (Poupaert and Couvreur, 2003). Semi-empirical PM3 and Density functional methods was used to carry out molecular calculations on the complexes. The structures were fully optimized and geometric calculations were done to obtain the bond length, bond angle, dihedrals and atomic charge distributions of the complexes. Thermodynamic calculations, vibrational frequencies, heat of formation, dipole moment, E-HOMO, E-LUMO, band gaps, heat of formation and polarizabilities were carried out (Fig. 2).

RESULTS AND DISCUSSION

Geometric calculations were carried out on the most stable structure using PM3 and DFT with B3LYP at 6-31G* level to obtain the bond length, bond angle, dihedral and atomic charge distribution. The bond length with PM3 method is between 1.92 and 1.49 while with DFT is 1.86 and 1.50. Bond angle is 111.32-70.59 with PM3 and 118.27-114.73 for Diethylamine dimethylglyoximate cobalt (II). For 2 aminophenol dimethylglyoxime Cobalt(II), the bond length is between 1.59-1.43 and with DFT it is between 1.43 to 1.49 and the bond angle is between 106.97 and 123.66 with PM3 and 116.83 and 121.23 with DFT. Lastly for Malonic acid dimethylglyoximate cobalt(II) the bond length is between 1.50 and 1.38, the bond angle is 104.04 and 87.24 with PM3 and 128.00 and 82.72. The values obtain for semi-empirical and ab-initio method differs by an order of magnitude for all the complexes as shown in Table 1-3.

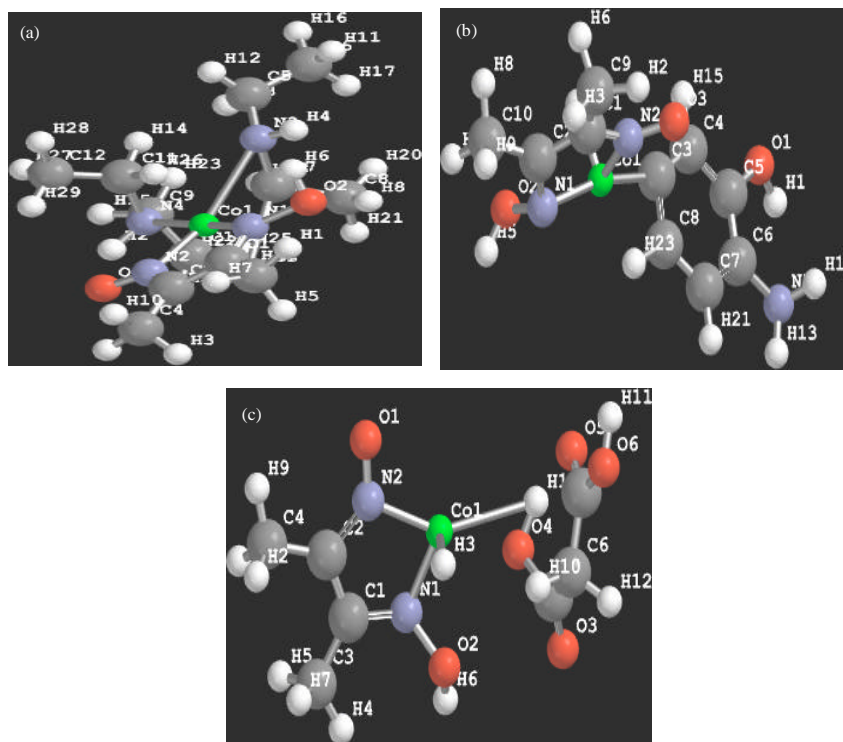


Fig. 2(a-c): (a) CoHdmg(dea)₂, (b) CoHdmg(2-aph) (c) CoHdmg(MO) and (a, b and c) Structures of the mixed ligands

Table 1: Selected bond length, bond angles and dihedrals of diethylamine dimethylglyoximate cobalt (II) (Å) angstromom

Bondlength	PM3	DFT/B3LYP	Bond Angle	PM3	DFT/B3LYP 6-31G*	Dihedrals	PM3	DFT/B3LYP6-31G*
Co-N ₂	1.92	1.86	Co-N ₂ -C ₄	111.32	118.27	Co-N ₃ -C ₅ -C ₄	5.06	-2.48
Co-N ₃	1.89	1.85	Co-N ₂ -O ₇	135.95	126.78	Co-N ₂ -C ₄ -C ₅	-4.81	0.55
Co-N ₉	2.62	2.01	Co-N ₃ -C ₅	113.19	116.59	Co-N ₂ -O ₇ -H ₈	72.71	-98.96
Co-N ₁₁	1.56	2.03	Co-N ₃ -O ₆	118.88	126.74	Co-N ₂ -C ₄ -C ₁₃	175.83	179.45
N ₂ -C ₄	1.34	1.33	Co-N ₉ -H ₁₀	118.09	109.18	Co-N ₃ -C ₅ -C ₁₇	-174.51	176.68
N ₂ -O ₇	1.49	1.44	Co-N ₉ -C ₂₁	135.78	109.52	Co-N ₉ -C ₂₁ -H ₂₂	88.01	50.09
N ₃ -C ₅	1.36	1.36	Co-N ₉ -C ₂₈	50.01	107.37	Co-N ₉ -C ₂₁ -H ₂₃	-26.32	-63.25
N ₃ -O ₆	6.24	1.29	Co-N ₁₁ -H ₁₂	106.47	98.47	Co-N ₉ -C ₂₁ -C ₂₄	-150.37	171.22
C ₄ -C ₅	1.44	1.42	Co-N ₁₁ -C ₃₅	136.09	114.39	Co-N ₉ -C ₂₁ -H ₂₉	110.96	74.60
C ₄ -C ₁₃	1.49	1.50	Co-N ₁₁ -C ₄₂	79.59	114.73	Co-N ₉ -C ₂₈ -H ₃₀	-17.71	-38.05

Table 2: Selected bonding distance, bonding angles and dihedrals of 2 aminophenol dimethylglyoxime Cobalt(II) (Å) angstromom

Bond length	PM3	DFT/B3LYP6-31G*	Bond angle	PM3	DFT/B3LYP 6-31G*	Dihedrals	PM3	DFT/B3LYP6-31G*
Co-H ₂	1.59	1.43	Co-N ₃ -C ₆	106.97	116.83	Co-N ₃ -C ₆ -C ₅	-31.22	6.81
Co-N ₃	1.88	1.83	Co-N ₃ -O ₂₁	93.89	125.19	Co-N ₄ -C ₅ -C ₆	3.31	0.33
Co-N ₄	1.81	1.90	Co-N ₄ -C ₅	109.33	116.08	Co-C ₇ -C ₈ -H ₉	0.48	4.64
Co-C ₇	1.93	1.87	H ₂ -Co-N ₃	94.17	96.53	Co-C ₇ -C ₈ -C ₁₀	-179.22	-175.17
N ₃ -C ₆	1.39	1.32	H ₂ -Co-N ₄	83.58	95.66	Co-C ₇ -C ₁₄ -C ₁₂	-177.77	173.63
N ₃ -O ₂₁	1.44	1.39	H ₂ -C ₀ -C ₇	95.93	91.81	Co-C ₇ -C ₁₄ -C ₁₅	-1.48	-8.55
N ₄ -C ₅	1.42	1.34	N ₃ -Co-H ₂	94.17	96.53	Co-N ₃ -O ₂₁ -H ₂₂	136.34	-27.02
N ₄ -O ₂₃	1.20	1.26	N ₃ -Co-N ₄	87.56	82.05	Co-N ₄ -C ₅ -C ₂₄	-173.79	-178.36
C ₅ -C ₆	1.39	1.44	N ₃ -Co-C ₇	164.36	103.92	Co-N ₃ -C ₆ -C ₂₈	151.54	-172.72
C ₅ -C ₂₄	1.48	1.49	N ₃ -C ₆ -C ₂₈	123.66	121.25	H ₂ -Co-N ₄ -C ₅	77.38	-93.31

Table 3: Selected bonding distances, bonding angles, and dihedrals of malonic acid dimethylglyoximate cobalt(II) (\AA) angstrom

Bond length	DFT/B3LYP6-31G*		Bond angle	DFT/B3LYP6-31G*		Dihedral	DFT/B3LYP6-31G*	
	PM3	DFT/B3LYP6-31G*		PM3	DFT/B3LYP6-31G*		PM3	DFT/B3LYP6-31G*
Co-H ₂	1.50	1.44	Co-N ₃ -O ₆	104.04	128.00	Co-N ₃ -O ₆ -H ₇	-139.33	-40.74
Co-N ₃	1.82	1.86	Co-N ₃ -C ₈	110.67	114.02	Co-N ₄ -C ₉ -C ₈	-2.85	1.94
Co-N ₄	1.84	1.75	Co-N ₄ -O ₅	114.74	101.48	Co-N ₃ -C ₉ -C ₈	15.79	7.09
Co-H ₁₈	2.38	2.74	Co-N ₄ -C ₉	113.03	121.83	Co-N ₃ -C ₈ -C ₁₀	-168.12	-172.47
N ₃ -O ₆	1.42	1.37	Co-H ₁₈ -O ₂₁	52.46	36.77	Co-N ₄ -C ₉ -C ₁₄	176.98	-176.14
N ₃ -C ₈	1.45	1.32	H ₂ -Co-N ₃	89.88	87.89	Co-H ₁₈ -O ₂₁ -C ₁₉	-131.32	-175.13
N ₄ -O ₅	1.19	1.26	H ₂ -Co-N ₄	86.75	89.39	H ₂ -Co-N ₄ -O ₅	99.03	99.56
N ₄ -C ₉	1.42	1.31	H ₂ -Co-H ₁₈	100.01	97.02	H ₂ -Co-N ₃ -O ₆	-54.42	-78.32
O ₆ -H ₇	0.95	0.98	N ₃ -Co-H ₂	89.876	87.89	H ₂ -Co-N ₃ -C ₈	72.99	84.79
C ₈ -C ₉	1.38	1.46	N ₃ -Co-N ₄	87.241	82.72	H ₂ -Co-N ₄ -C ₉	-80.33	-86.54

Table 4: Electronic properties of the complexes

COMPLEXES/	Dipole moment (debye)		EHOMO (eV)		ELUMO (eV)		Bandgap (eV)	
	PM3	DFT	PM3	DFT	PM3	DFT	PM3	DFT
CoHdmg (dea) ₂	4.50	6.39	-8.34	-3.28	0.34	0.54	8.68	3.82
CoHdmg (2aph)	4.83	5.06	-8.81	-5.47	-1.38	-2.58	7.34	2.91
CoHdmg (MO)	0.98	4.30	13.94	9.70	-6.12	-6.51	7.82	3.19

Table 5 : Thermodynamic properties of the cobalt(II) complexes

Complex	Methods	Heat of formation kJ mol ⁻¹	SCF Total energy (au)	Free energy (au)	Enthalpy (au)	Entropy Jmol ⁻¹ k ⁻¹
CoHdmg (dea) ₂	PM3	-7082.63	-	-2.321	-2.255	577.09
	DFT/6-31G*	-	-2226.76	-2226.38	-2226.31	606.36
CoHdmg (2aph)	PM3	-6713.83	-	-2.355	-2.298	501.27
	DFT/6-31G*	-	-2161.90	-2161.71	-2161.65	514.59
CoHdmg (MO)	PM3	-6554.89	-	-2216.978	-2216.921	504.39
	DFT/6-31G*	-	-2474.791	-2474.628	-2474.570	509.21

Electronic properties: The electronic properties of the structures were described by their bands (Young, 2001). The HOMO-LUMO band gaps were calculated using PM3 and DFT/B3LYP/6-31G* method. The value obtained for PM3 is greater than that of DFT/B3LYP/6-31G*, for all the complexes that is for CoHdmg (2aph) is +7.34 eV, CoHdmg (dea)₂ is +8.68 eV and CoHdmg (MO) is +7.82 for PM3 and for DFT method, the values are +7.34, +3.82 and +3.19, respectively. This shows that PM3 method predict the electronic properties better than the DFT/B3LYP/6-31G* method as shown in Table 4.

Thermodynamic properties and stabilities: Complexes are thermodynamically stable if ΔG and ΔH are negative. The more negative ΔG and ΔH , the more positive ΔS is and the most stable the complex becomes. From Table 5 negative values of ΔH , ΔG and positive ΔS obtained that is for CoHdmg (2aph) PM3 (-2.29 au, -2.35 au, 501.27 J mol⁻¹ k⁻¹) DFT/B3LYP/6-31G* (-2161.65 au, -2161.71 au, 514.59 J mol⁻¹ k⁻¹), CoHdmg(dea) PM3 (-2.25 au, -2.32 au, 577.09 J mol⁻¹ k⁻¹), DFT/B3LYP/6-31G* (-2161.65 au, -2161.71 au, 514.59 J mol⁻¹ k⁻¹) and CoHdmg (MO) PM3 (-2216.92 au, -2216.98 au, 504.39 J mol⁻¹ k⁻¹), DFT/B3LYP/6-31G* (-2474.57 au, -2474.63 au and 509.21 J mol⁻¹ k⁻¹). Calculation with DFT/B3LYP/6-31G* basis set better predicts the stability of the Dimethylglyoxime Co(II), complexes.

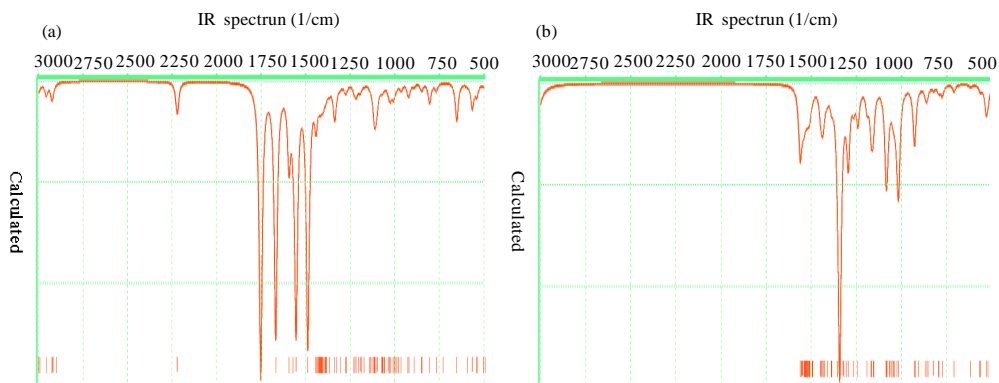
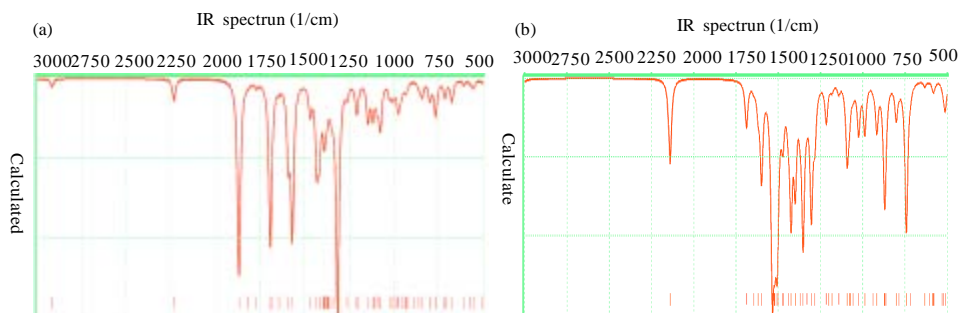
Fig. 3(a-b): (a) CoHdmg(dea)₂ with PM3 and (b) With DFT/B3LYP/6-31G*

Fig. 4(a-b): (a) CoHdmg(2-aph) with PM3 and (b) With DFT/B3LYP/6-31G*

Vibrational frequencies: The vibrational frequencies obtained from theoretical calculations were in agreement with the experimental data reported (Osunlaja *et al.*, 2009) as shown in Table 6 and their corresponding infra red spectra as shown in Fig. 3a,b, 4a,b and 5a, b. It was observed that the values obtained from PM3 is closer to experimental values than the DFT/B3LYP/6-31G* values. For instance, CoHdmg (2aph) $\eta(\text{N-H})_{\text{str}}$ the experimental result is 3154 cm^{-1} while the theoretical calculation, PM3 (3394 and 3523 cm^{-1}), DFT/B3LYP/6-31G* (3549 - 3467 cm^{-1}), $(\text{O-H})_{\text{str}}$ experimental 3381 cm^{-1} , theoretical calculation, PM3(3874 - 3886 cm^{-1}) and DFT/B3LYP/6-31G* (3540 - 3520 cm^{-1}). (Co-N) , the experimental is 507 cm^{-1} , PM3 (643 cm^{-1}), DFT/B3LYP/6-31G* (360 cm^{-1}) and for $(\text{N-O})_{\text{str}}$, the experimental value is 115 cm^{-1} while with PM3 (1869 cm^{-1}), DFT/B3LYP/6-31G* (1619 cm^{-1}).

For CoHdmg(dea)₂, $(\text{O-H})_{\text{str}}$ the experimental value is 3430 cm^{-1} while the theoretical calculation, PM3 (3901 cm^{-1}), DFT/B3LYP/6-31G* (3647 cm^{-1}), $(\text{N-H})_{\text{str}}$ the experimental result is 3174 cm^{-1} while the theoretical calculation, PM3 is 3320 - 3044 cm^{-1} and DFT/B3LYP/6-31G* (3439 - 3320 cm^{-1}). $(\text{C} = \text{N})_{\text{str}}$ the experimental data is 1462 cm^{-1} , PM3 (1752 cm^{-1}), DFT/B3LYP/6-31G* (1538 cm^{-1}). $(\text{N-O})_{\text{str}}$ experimental is 1206 cm^{-1} , with PM3 (1668 cm^{-1}), DFT/B3LYP/6-31G* (1449 cm^{-1}). (Co-N) experimental is 510 cm^{-1} , with PM3 (535 cm^{-1}), DFT/B3LYP/6-31G* (563 cm^{-1}).

For CoHdmg(MO), $(\text{O-H})_{\text{str}}$ experimental is 3403 cm^{-1} while theoretical calculation with PM (3858 - 3815 cm^{-1}) and DFT/B3LYP/6-31G* (3647 - 3545 cm^{-1}). $(\text{C} = \text{O})_{\text{carboxylic}}$ in the experimental result is 1591 cm^{-1} , theoretical calculation, PM3 (1903 cm^{-1}),

Table 6: Experimental and theoretical Infra red data showing absorption bands with their corresponding vibration for the cobalt II complexes

Complexes	Bond	Experimental	PM3	DFT/B3LYP/6-31G*
CoHdmg (dea)2	O-H stretch	3430	3901	3647
	N-Hstretch	3174	3320-3044	3439-3320
	C = Nstretch	1462	1752	1538
	N-Ostretch	1206	1668	1449
	Co-Nstretch	510	535	563
	O-Hbend	N/A	1367-1337	1343-1324
	C-Hstretch	N/A	3182-3175	3162-3155
	C-Cstretch	N/A	1593-1554	1562-1490
CoHdmg (2aph)	N-H stretch	3154	3394 and 3523	3549-3467
	O-H stretch	3381	3874-3886	3549-3520
	Co-N stretch	507	643	360
	N-Ostretch	1154	1869	1619
	C-H stretch	N/A	3161 and 3155	3171-3157
	Co- H stretch	N/A	2916-1007	2140
	C-H unsaturation	N/A	3083 and 3063	3125-3063
	C = C stretch	N/A	1771-1593	1080
CoHdmg (MO)	C-C stretch	N/A	1693-1571	1538
	O-H stretch	3403	3858-3815	3647-3545
	C = O stretch	1591	1903	1875-1222
	N-O stretch	1080	1937	1617
	O-H stretch	1336	2059	2540-1875
	Co-N stretch	510	1422	1002
	C-H saturation	N/A	3143-1376	3132
	Co-H stretch	N/A	3340-2946	2540-2167
	C-C stretch	N/A	1746	1511-1506
	C-N stretch	N/A	964	1651
	C-Hstretch	N/A	2995-2912	3118-3080

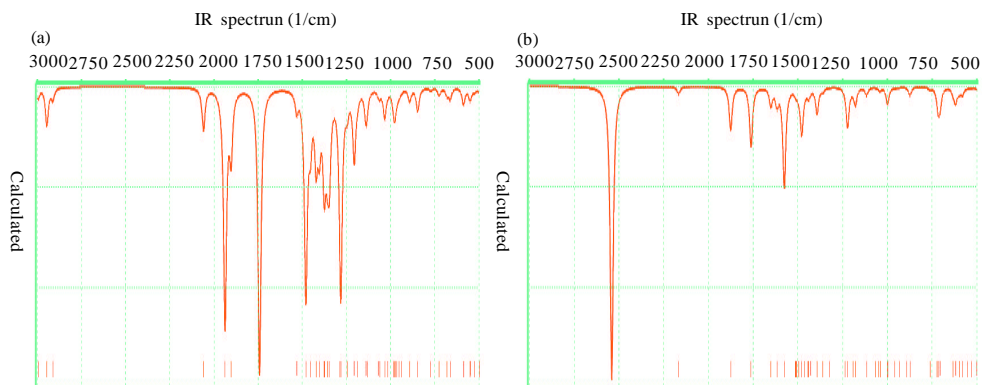


Fig. 5(a-b): (a) CoHdmg(MO) with PM3 and (b) With DFT/B3LYP/6-31G*

DFT/B3LYP/6-31G* (1875-1222 cm^{-1}). $(\text{N-O})_{\text{str}}$, experimental result is 1080 cm^{-1} , PM3 (1937 cm^{-1}), DFT/B3LYP/6-31G* (1617 cm^{-1}). $(\text{C} = \text{O})_{\text{str}}$ experimental is 1336 cm^{-1} and PM3 (2059 cm^{-1}),

Table 7: Wavelength and intensity of dethylamine dimethylglyoxime cobalt(II)

CoHdmg (dea) ₂		CoHdmg (2aph)		CoHdmg (MO)	
Wavelength (nm)	Intensity	Wavelength (nm)	Intensity	Wavelength (nm)	Intensity
466.47	0.0162056	463.73	0.004	431.28	0.001
484.54	0.00675398	497.42	0.019	450.83	0.003
535.54	0.00257569	568.90	0.001	463.82	0.003
643.60	0.000389802	650.23	0.013	570.17	0.007
1076.84	0.000251827	711.91	0.011	633.86	0.001
1094.90	0.000320453	987.78	0.0002	812.49	0.0002

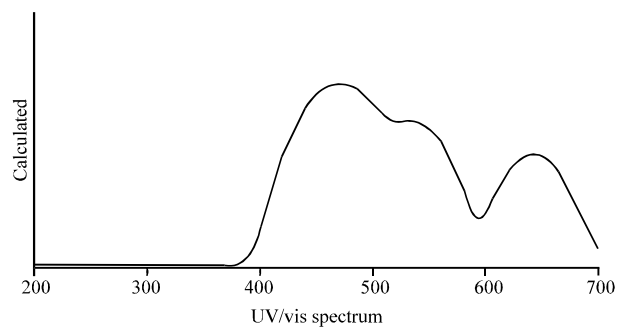


Fig. 6: UV/visible spectra of Dethylamine Dimethylglyoxime Cobalt (II)with DFT/B3LYP/6-31G*

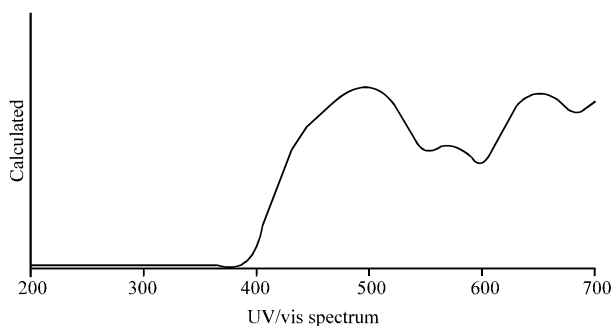


Fig. 7: Ultra-violet/visible spectra of 2 aminophenol Dimethylglyoxime Cobalt (II) with DFT/B3LYP/6-31G*

DFT/B3LYP/6-31G* (2540-1875 cm^{-1}). (Co-N)_{str} experimental is 510 cm^{-1} while PM3 (1422 cm^{-1}), DFT/B3LYP/6 31G* (1002 cm^{-1}).

Electronic spectra using Uv/visible: The Uv/visible spectra data (Table 7) showed three major absorption bands. These bands are due to intra-ligand, metal-ligand charge transfer and d-d transitions within the metal complexes. The uv/visible spectrum of CoHdmg (dea)₂ showed (Fig. 6) well resolved absorption bands at 467, 485 nm, these transitions are attributed to metal-ligand charge transfer transitions while the band at 535 nm is assigned to d-d transition within the metal. The uv/visible spectrum of CoHdmg (2aph) (Fig. 7) presents three distinct bands at 497, 650 nm attributed to metal-ligand charge transition while the band at 650 nm may account for d-d transition with d-orbital of the metal ion. Likewise the three prominent bands in the uv/visible

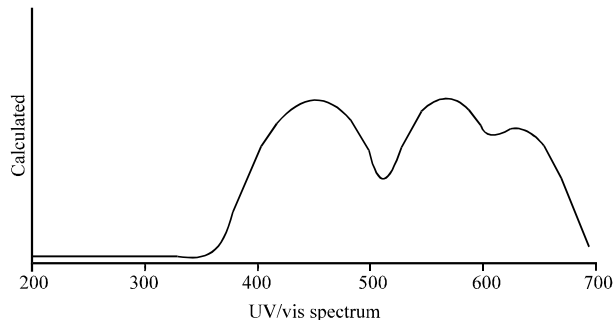


Fig. 8: Ultra-violet/visible spectra of Malonic acid Dimethylglyoxime Cobalt(II) with DFT/B3LYP/6-31G*

spectrum of CoHdgm (MO) (Fig. 8) at 451, 463 nm are metal-ligand charge transfer transitions while the band at 570 nm is attributed to the d-d transition within the d-orbitals of the metal ion.

CONCLUSION

The properties of the Complex [Co(II) mixed-ligand complexes of dimethylglyoxime] were calculated using Semi-empirical PM3 and DFT with B3LYP at 6-31G* level. The optimized geometries, dipole moments, geometric parameters, thermodynamics parameters and vibrational and electronic frequencies 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 results. It has also given us the opportunity to compute results on the properties that cannot be obtained in laboratory experiments. It can be concluded that in studying and predicting the geometric parameters and vibrational frequencies of these complexes, the PM3 semi-empirical calculation is the best though it did not account for the chemical shifts which was accounted for by the DFT/B3LYP/6-31G*.

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