Supporting Information

Figure S1	Synthesis of benzimidazole ligand L
Figure S2	ATR spectra of a) L, b) **1**, c) **2** and d) **3**.
Figure S3	ESI-MS(+) spectrum of **3**.
Figure S4	Absorption spectra of complexes (a) **1**, (b) **2** and (c) **3** in DMF.
Figure S5	TG and DTG curves of complexes **1–3**.
Figure S6	Calculated electronic spectra of the complexes studied here (a) **1**, (b) **2** and (c) **3** CAM-B3LYP/LANL2DZ method.
Figure S7	Selected FMO orbitals of mononuclear analogue of **1.**
Figure S8	Selected FMO orbitals of mononuclear analogue of **2.**
Figure S9	Selected FMO orbitals of mononuclear analogue of **3.**
Table S1	Selected bond lengths (A), and angles (^{o}) for **1–3** obtained at the B3LYP/LANL2DZ theory level.
Table S2	Selected Mulliken charge values of the mononuclear models of **1–3.**

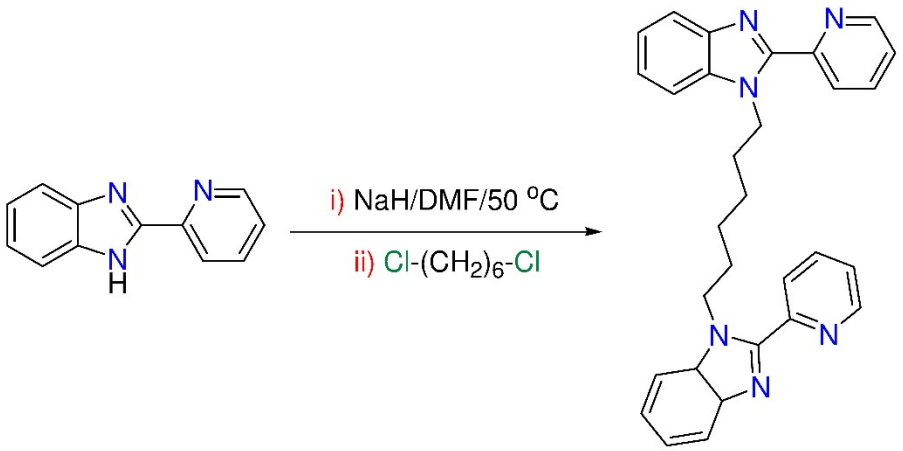
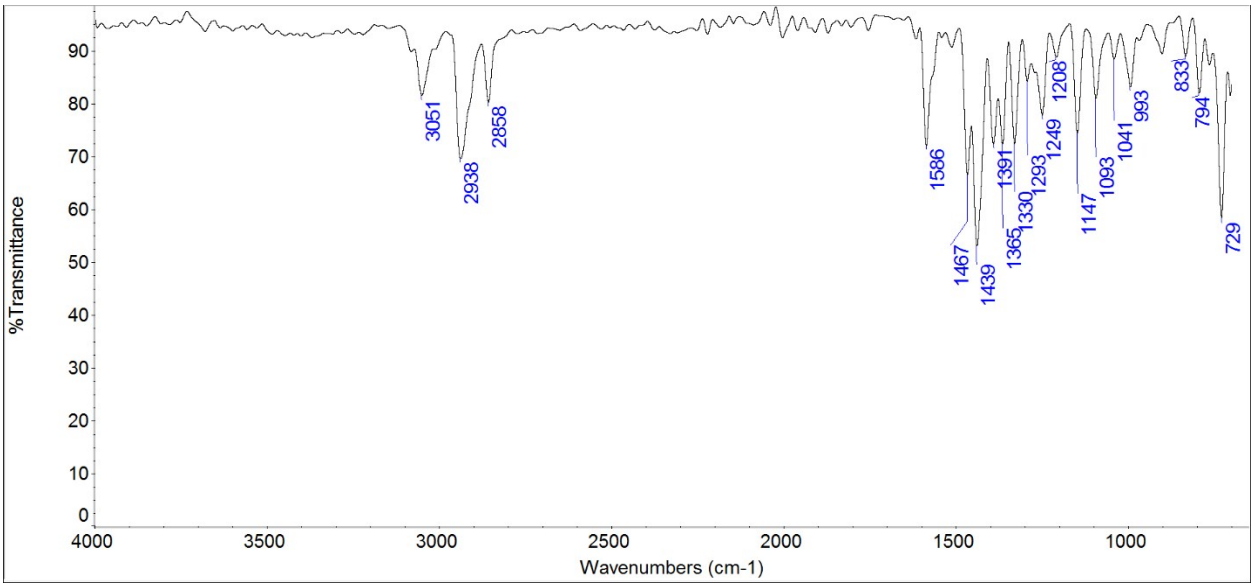
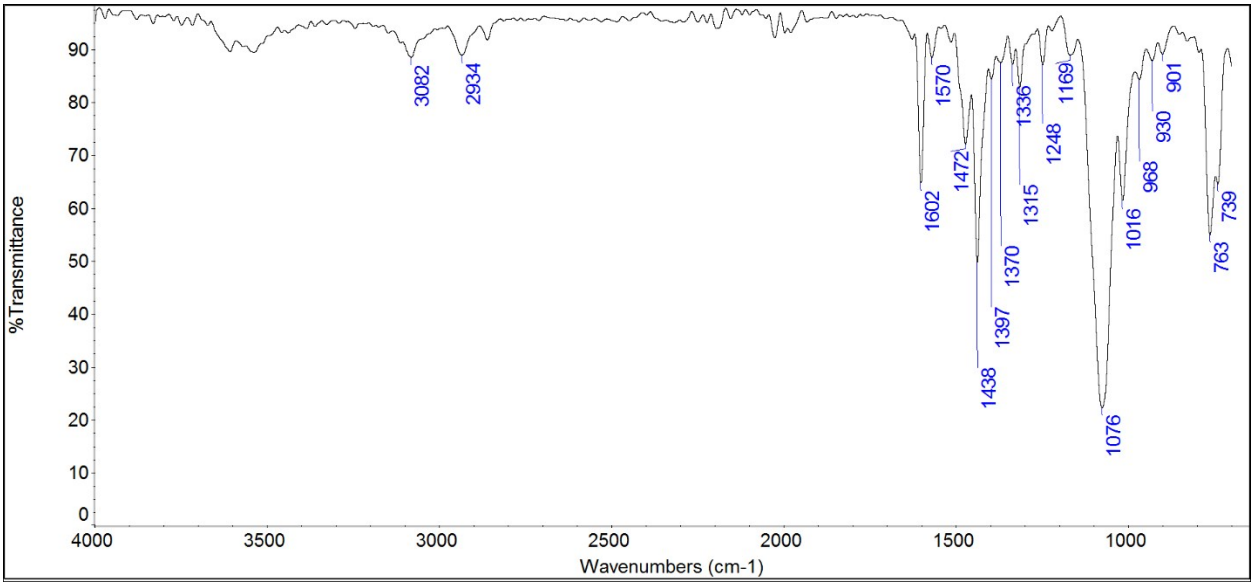


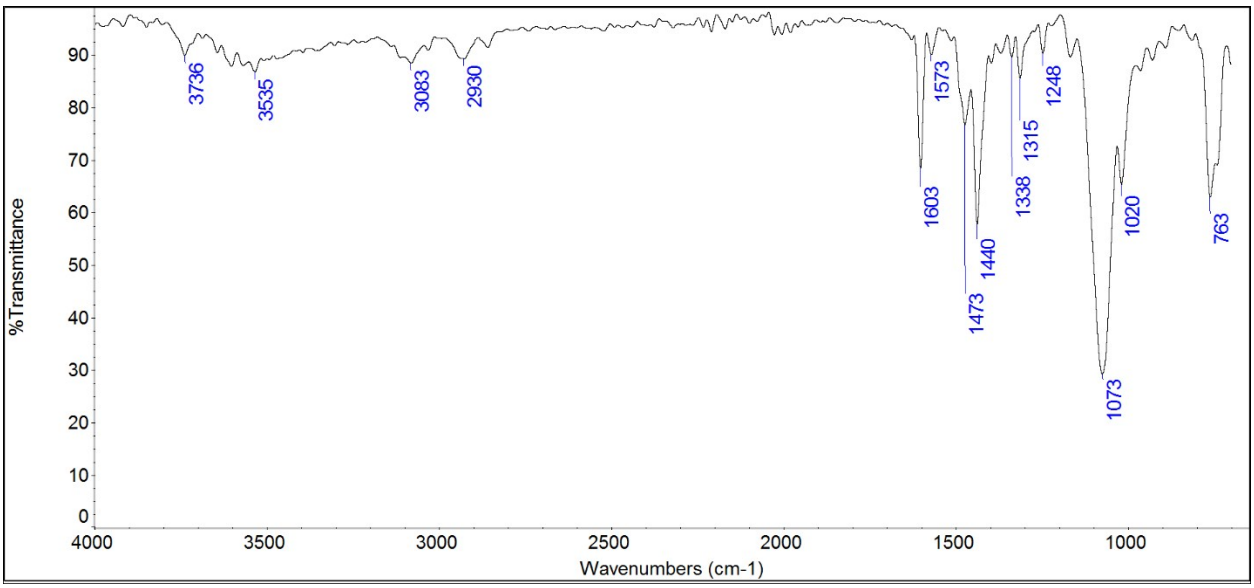
Figure S1 Synthesis of benzimidazole ligand L.[15]


%Transmittance
Wavenumbers (cm-1)
3051
2938
2858
1586
1467
1439
1391
1365
1330
1293
1249
1208
1147
1093
1041
993
833
794
729

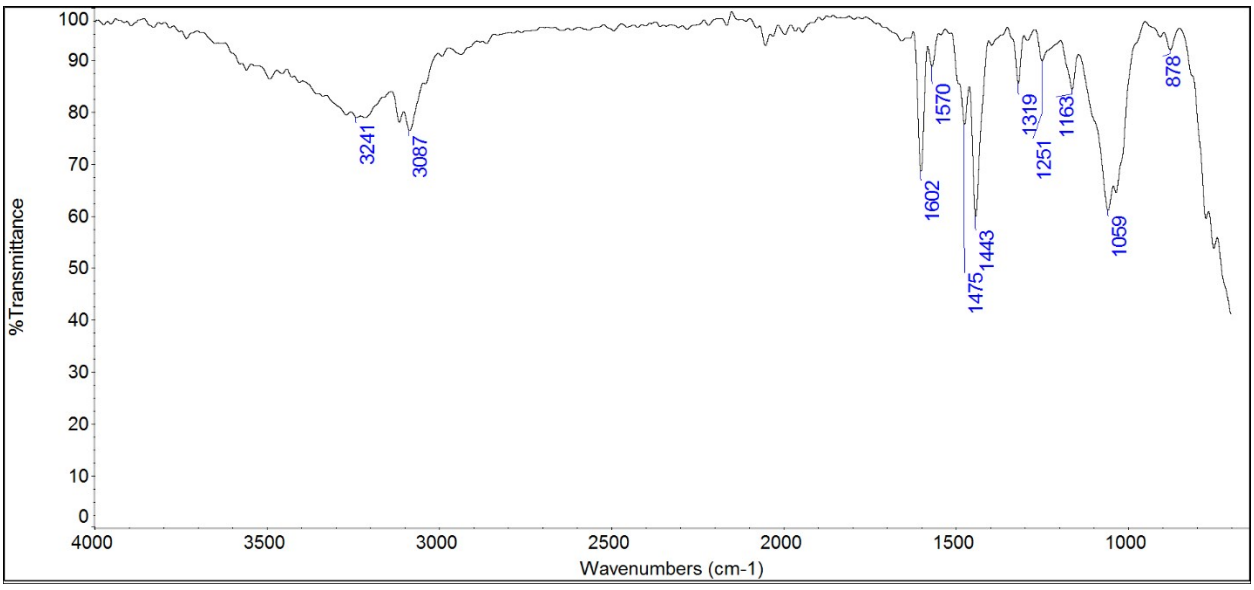
a)


%Transmittance
Wavenumbers (cm-1)
3082
2934
1602
1570
1472
1438
1397
1370
1336
1315
1248
1169
1076
1016
968
930
901
763
739

b)



c)



d)

Figure S2 ATR spectra of a) L, b) **1**, c) **2** and d) **3**.

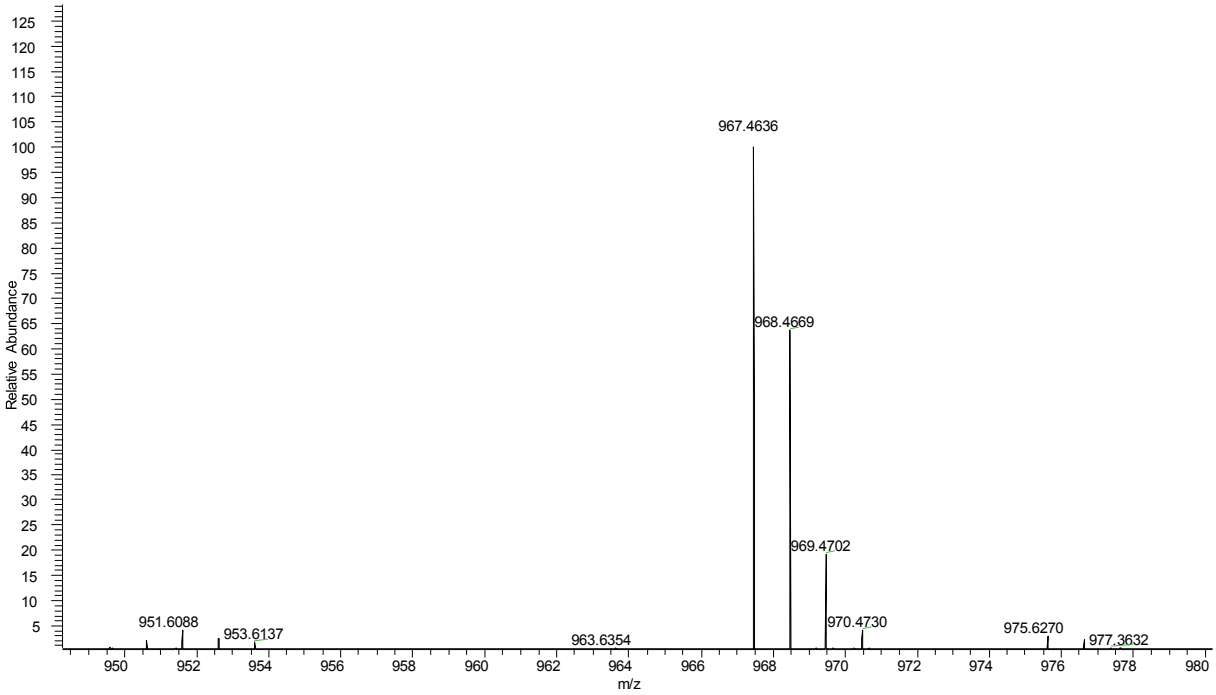


Figure S3 ESI-MS(+) spectrum of **3**.

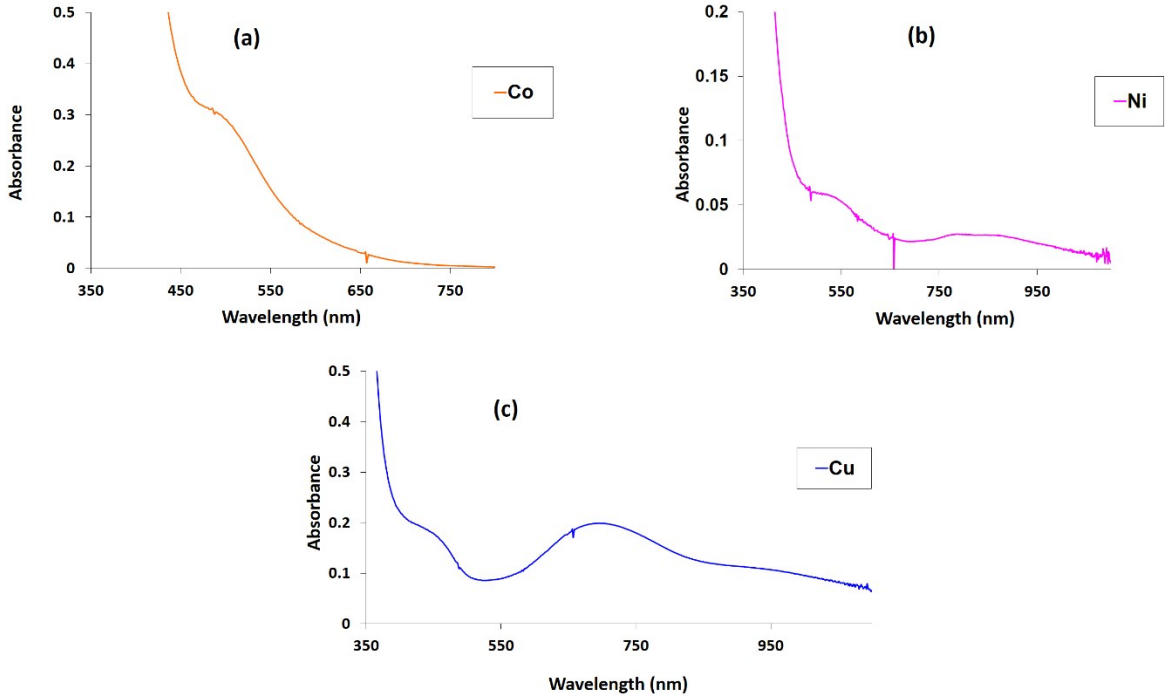


Figure S4 Absorption spectra of complexes (a) **1**, (b) **2** and (c) **3** in DMF.

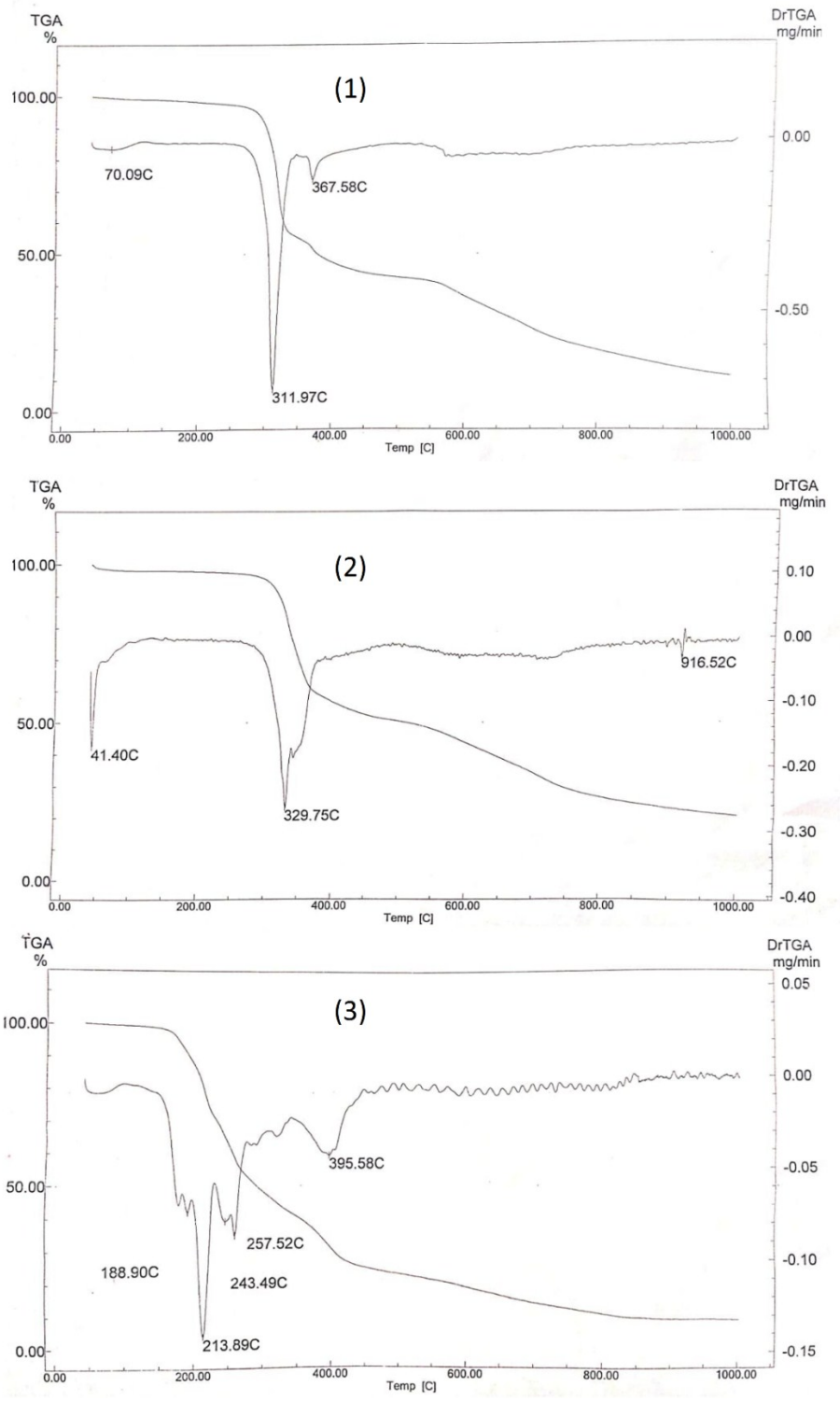


Figure S5 TG and DTG curves of complexes **1**–**3**.

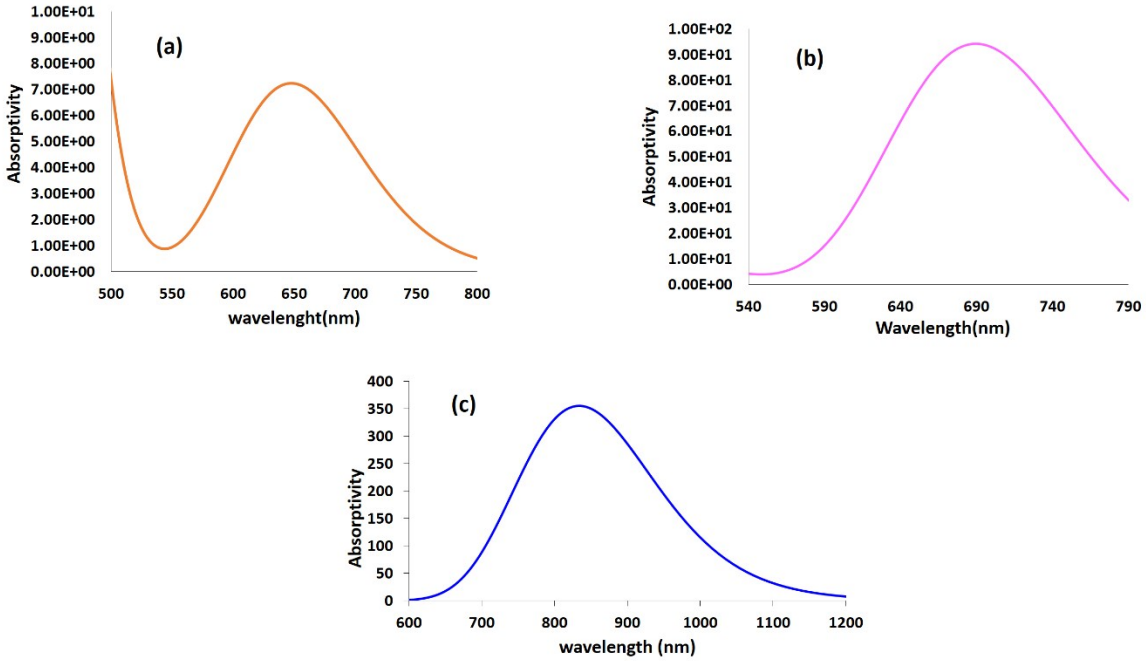


Figure S6 Calculated electronic spectra of the complexes studied here (a) **1**, (b) **2** and (c) **3** CAM-B3LYP/LANL2DZ method.

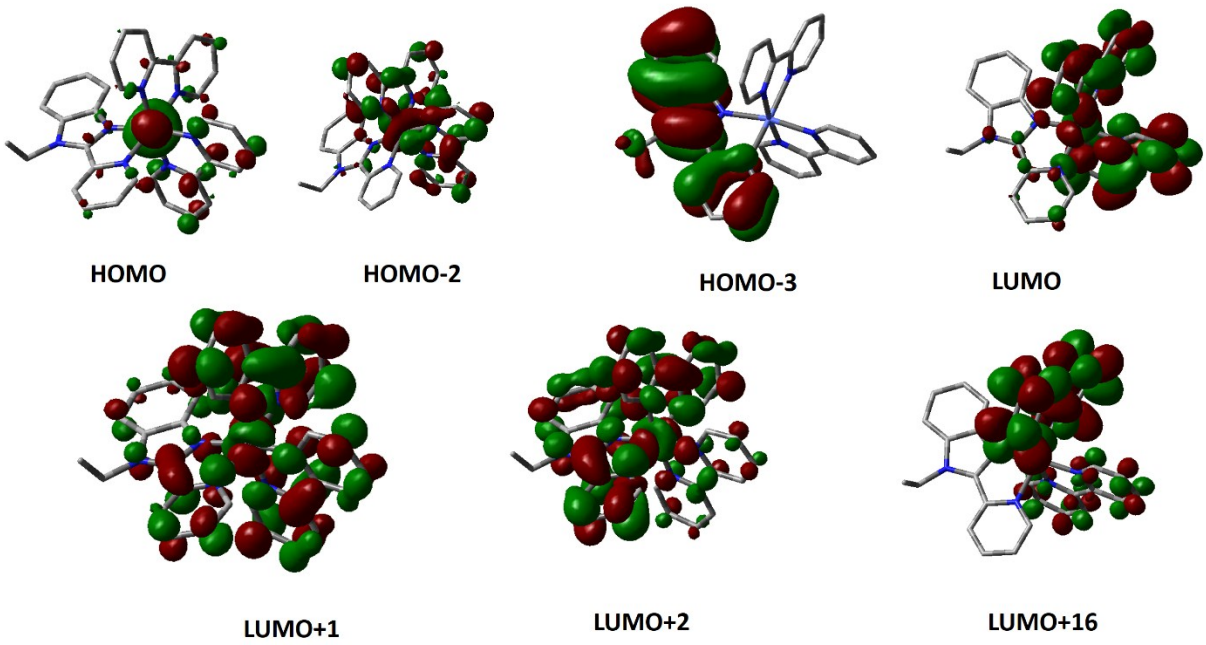


Figure S7 Selected FMO orbitals of mononuclear analogue of **1.**

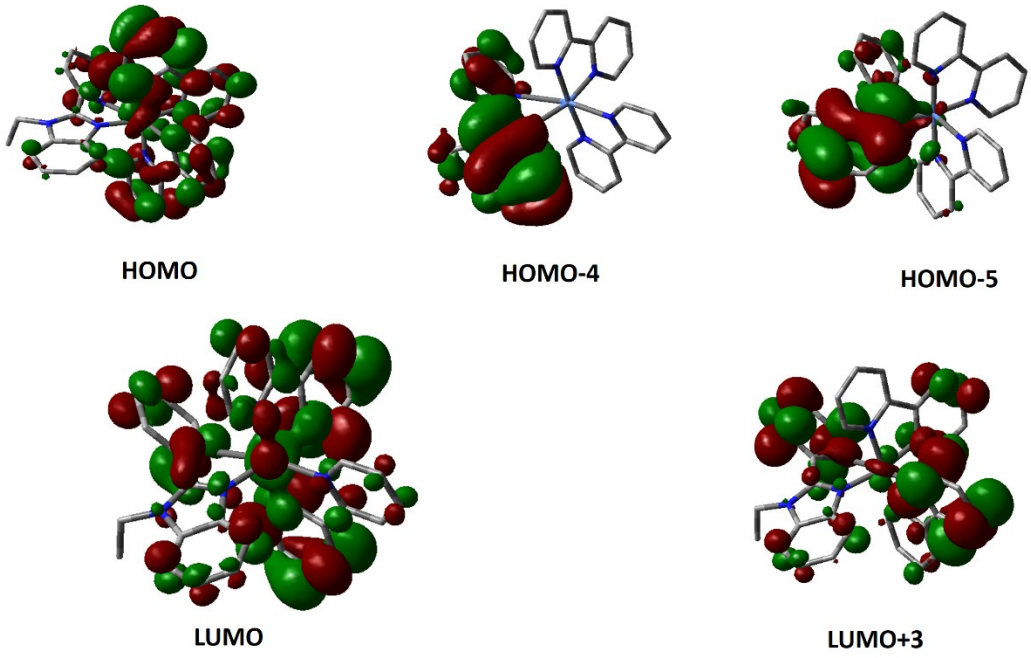


Figure S8 Selected FMO orbitals of mononuclear analogue of **2.**

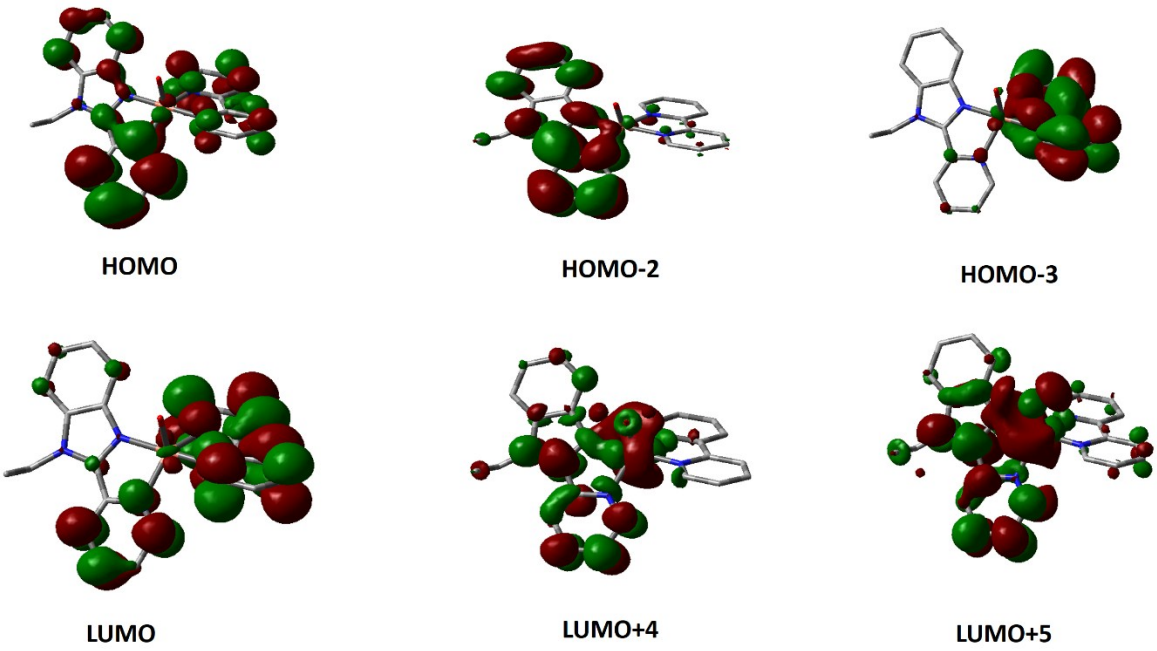


Figure S9 Selected FMO orbitals of mononuclear analogue of **3**

Table S1 Selected bond lengths (A), and angles (°) for **1–3** obtained at the B3LYP/LANL2DZ theory level.

1		**2**		**3**	
Bond length (A°)	**Bond angle (°)**	**Bond length (A°)**	**Bond angle (°)**	**Bond length (A°)**	**Bond angle(°)**
Co–N1= 2.277	N2–Co–N67 = 169.85 N1–Co–N69 = 175.99 N68–Co–N70 = 173.19 N68–Co–N67 = 81.99	Ni–N1= 3.165	N68– Ni –N67= 83.23 N1–Ni –N69= 167.55 N2–Co–N67 =159.69 N68–Co–N70=175.82	Cu–N1= 2.132	N1–Cu–N2=79.76 N49–Cu–N50=80.86 N1–Cu–N49=100.57
Co–N2 = 1.998	N2–Co–N70 = 89.27	Ni–N2= 1.951	N2–Ni–N70= 89.63	Cu–N2= 1.973	O52–Cu–N2=88.24
Co–N67 = 1.997	N69–Co–N67 = 87.96	Ni–N67= 1.974	N69–Ni–N67= 90.45	Cu–N49= 2.005	O52–Cu–N1=115.65
Co–N68 = 1.991	N1–Co–N68 = 89.11	Ni–N68= 1.928	N1– Ni –N68= 94.016	Cu–N50=2.079	O52–Cu–N50=118.82
Co–N69 = 2.222	N1–Co–N2 = 77.21	Ni–N69= 2.377	N1– Ni –N2= 68.30	Cu–O= 2.191	O52–Cu–N49=88.53
Co–N70 = 2.005		Co–N70= 1.937			N50–Cu–N2=101.78

Table S2 Selected Mulliken charge values of the mononuclear models of **1–3.**					
1		**2**		**3**	
N(1)	-0.155821	N(1)	-0.100372	N(1)	-0.269480
N(2)	-0.281633	N(2)	-0.343720	N(2)	-0.380299
N(67)	-0.220799	N(67)	-0.223615	N(49)	-0.305435
N(68)	-0.223691	N(68)	-0.254231	N(50)	-0.291107
N(69)	-0.172202	N(69)	-0.133946	O(52)	-0.713220
N(70)	-0.234979	N(70)	-0.280498	Cu(II)	0.711931
Co(II)	0.430933	Ni(II)	0.464320		