Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Twisted conformations in complexes of N-(3-imidazol-1-yl-propyl)-1,8-naphthalimide and fluorescence properties

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Table 1S: Absorption and emission of complexes [#] **1-7**

Complex / ligand	Absorption in solid (nm)	Emission in solid (nm)
L	361	461
1	315, 353	428
2	330	425
3	318, 351	426
4	323	470
5	361	452
6	357	473
7	360	481

Table 2S : The quantum yield of the complexes determined in DMF solution

S.I No.	Compound	Quantum yield
1	Ligand, **L**	0.36
2	Complex **1**	0.37
3	Complex **2**	0.35
4	Complex **3**	0.40
5	Complex **4**	0.38
6	Complex **5**	0.41
7	Complex **6**	0.50
8	Complex **7**	0.46

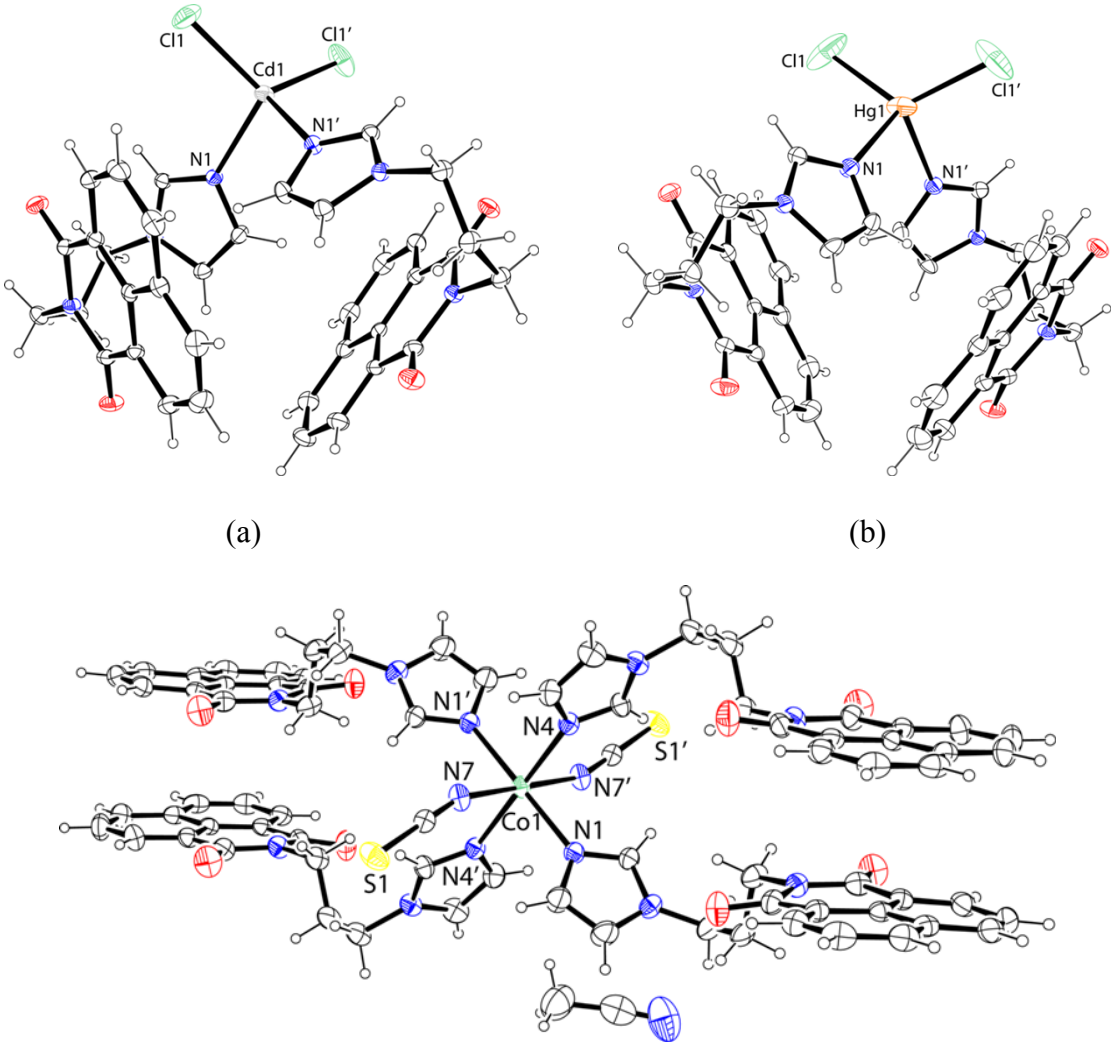


Figure 1S: ORTEP diagram of (a) complex **2**, (b) complex **3**, (c) complex **5** (symmetry of equivalent atoms x,-y,-z)

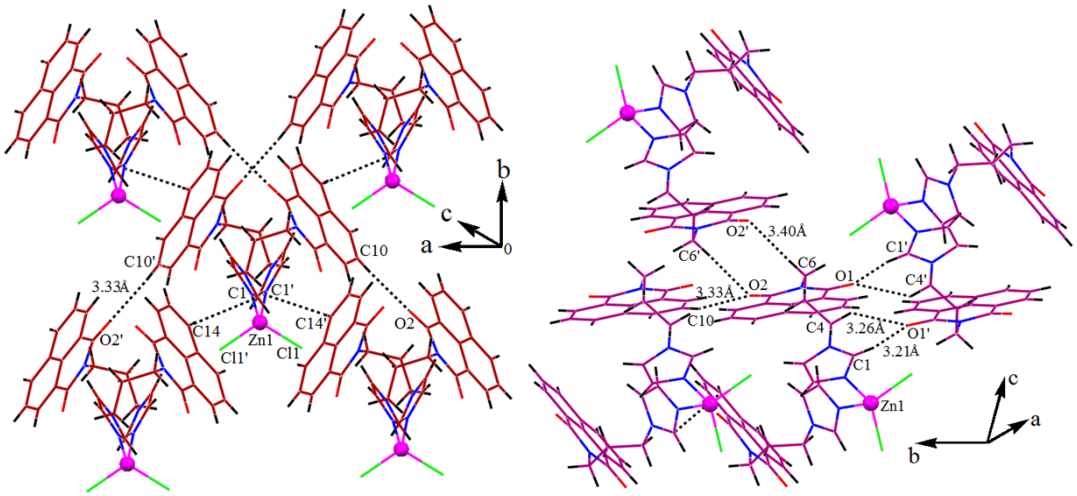


Figure 2S: Weak interactions in the crystal lattice of the complex **1** from two different projections.

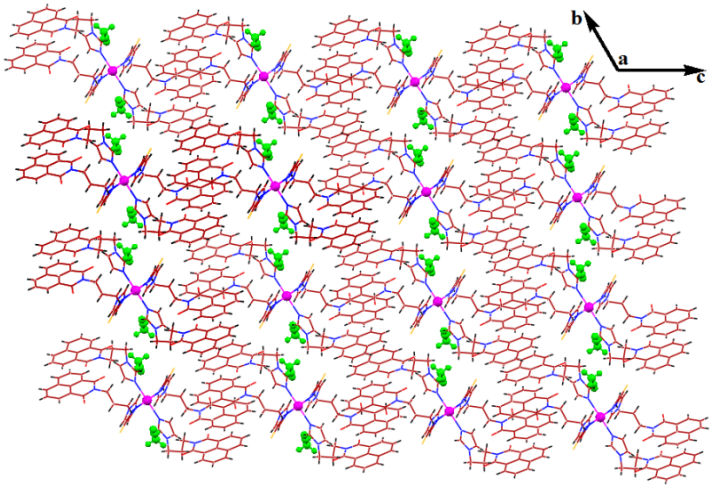


Figure 3S: 3D supramolecular network along a-axis. in the lattice of complex **4**.

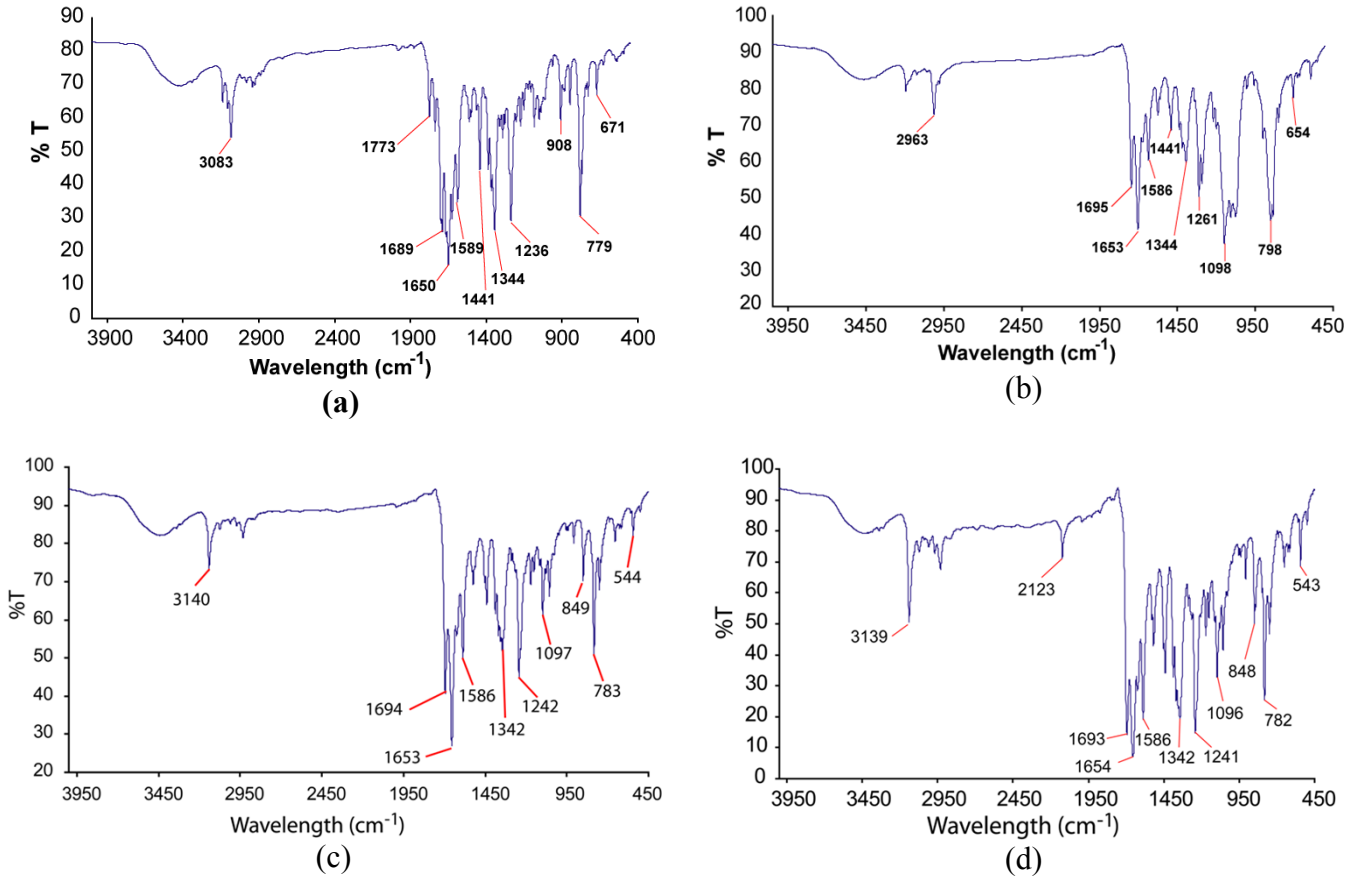


Figure 4S1: FT-IR (KBr) spectra of the (a) ligand, **L**, (b) Complex **1,** (c) Complex **2,** (d) Complex **3.**

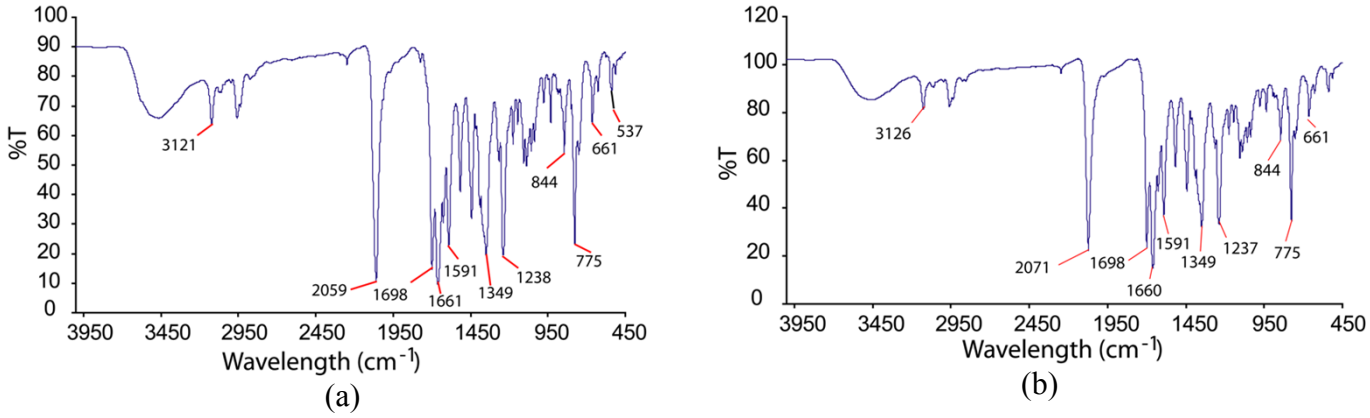
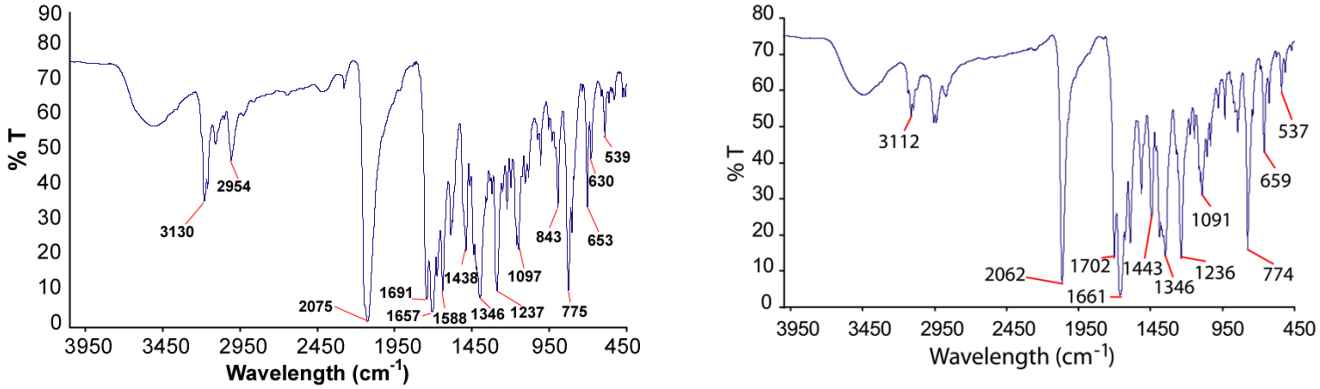


Figure 4S2: FT-IR spectra (KBr) of the (a) Complex **4** and (b) Complex **5.**



(a) (b)

Figure 4S3: FT-IR spectra (KBr) of the (a) complex **6** and (b) Complex **7**

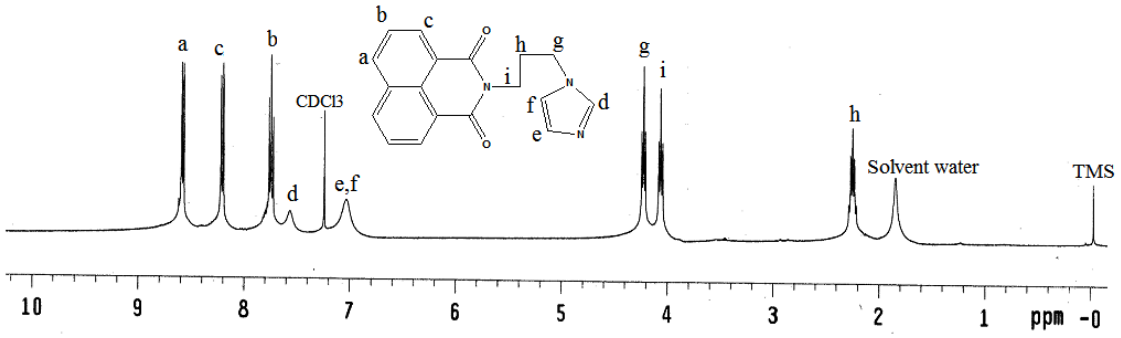


Figure 5S: ^{1}HNMR (400MHz, $CDCl_3$) spectrum of the ligand, **L**

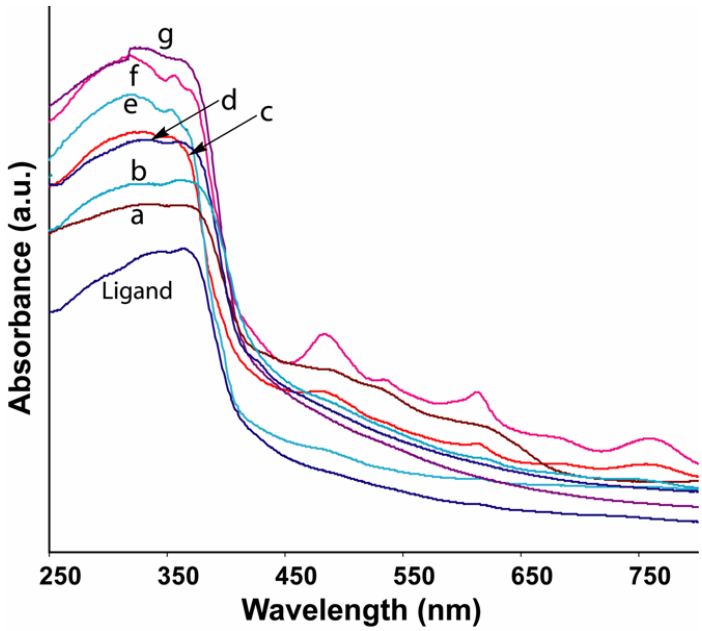


Figure 6S: Solid state UV-vis spectra of (a) complex **5**, (b) complex **7**, (c) complex 6, (d) complex **2**, (e) complex **3**, (f) complex **1**, and (g) complex **4**.

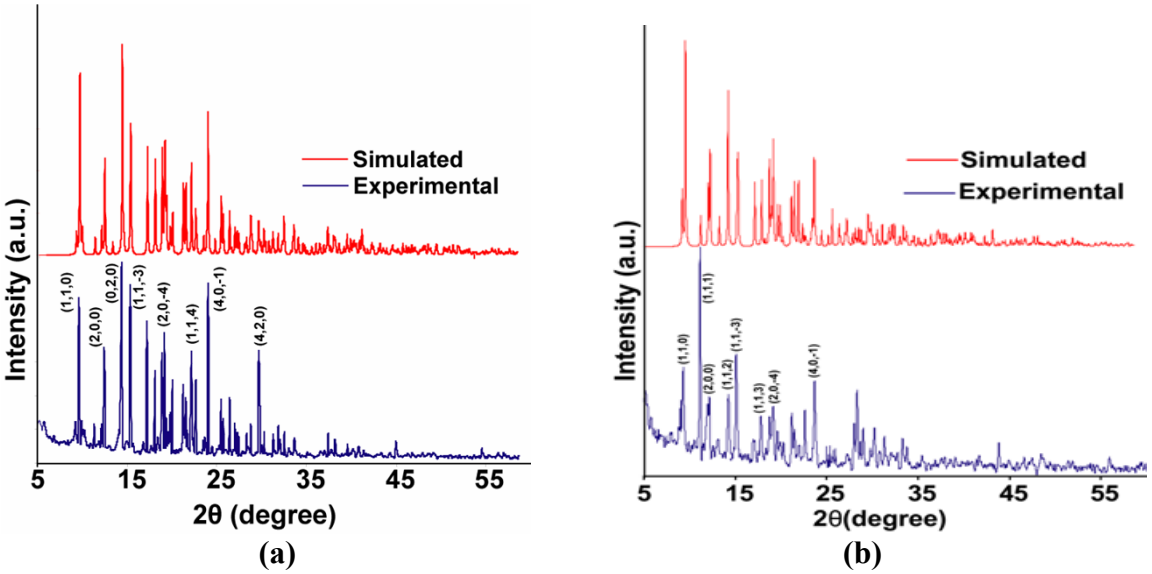


Figure 7S: PXRD pattern of the (a) complex **2** and (b) Complex **3**

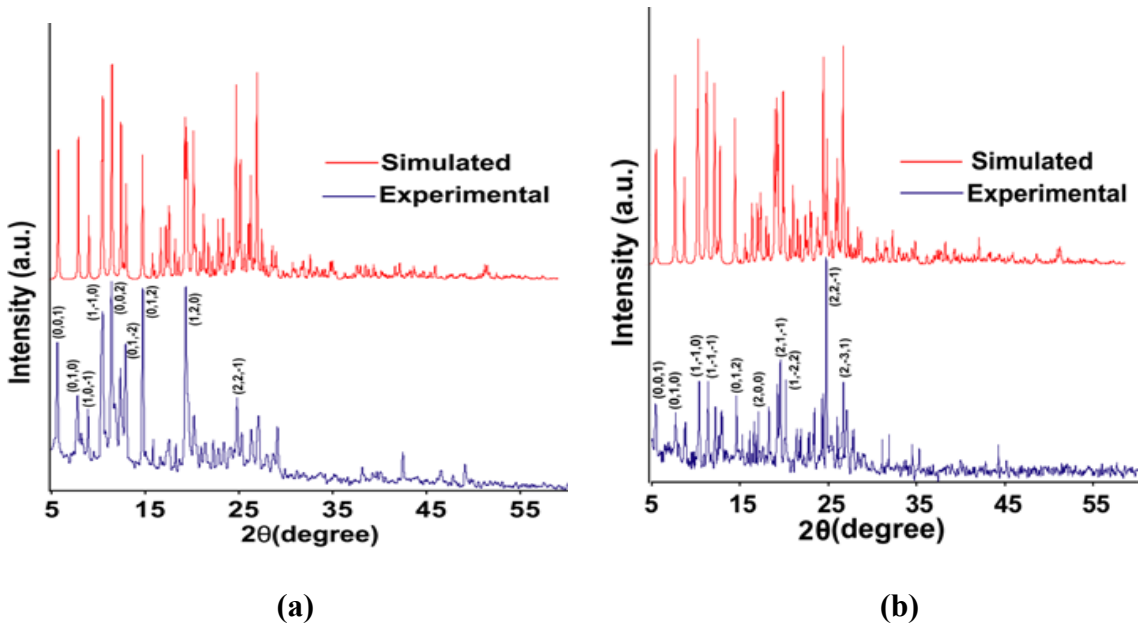


Figure 8S: PXRD pattern of the (a) complex **4** and (b) Complex **5**

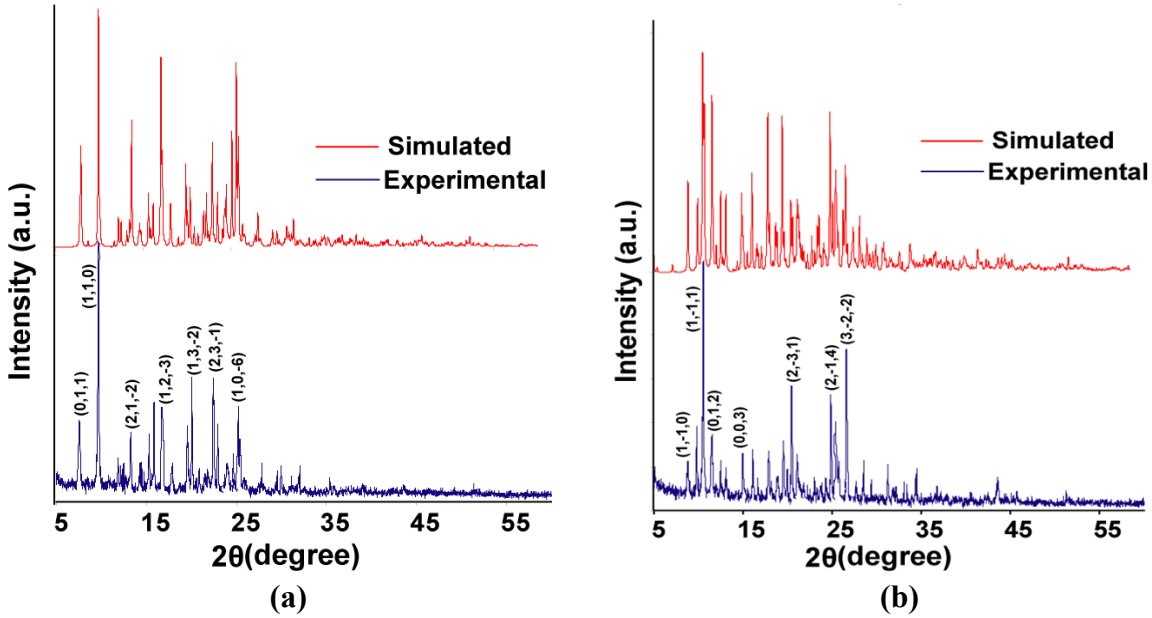


Figure 9S: PXRD pattern of the (a) complex **6** and (b) complex 7

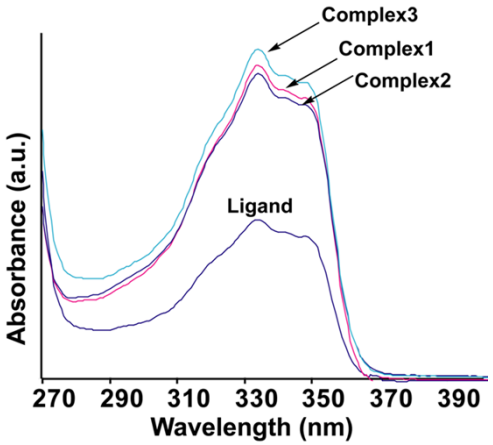


Figure 10S : UV-Vis spectra of the ligand, complex **1**, complex **2** and complex **3** in DMF (concentration of 10^{-6}M each)

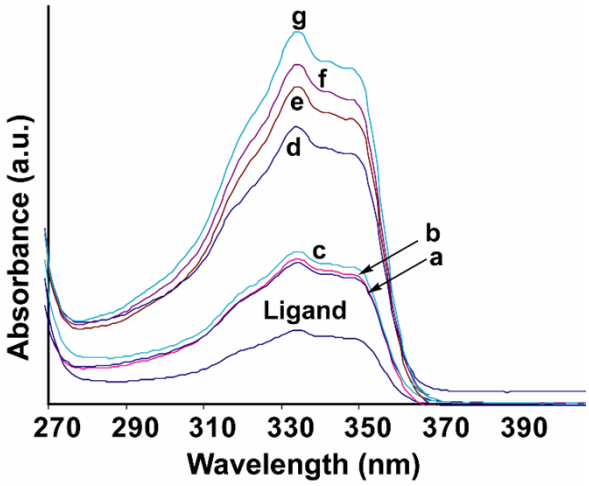


Figure 11S: UV-Vis spectra of the ligand, (a) complex **2**; (b) complex **1**; (c) complex **3**; (d) complex **6**; (e) complex **5**; (f) complex **4**; (g) complex **7**; in DMF (concentration of 10^{-6}M each).

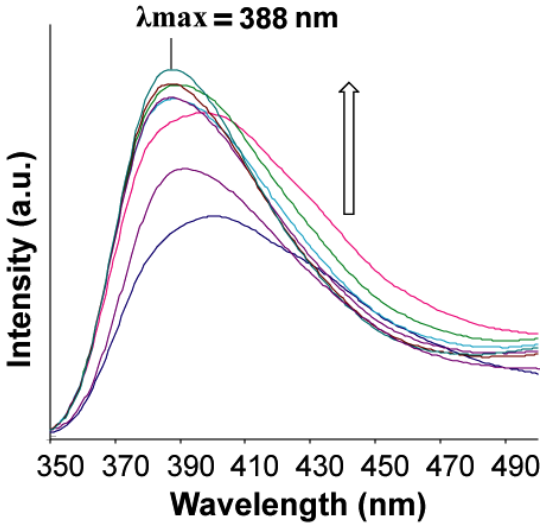


Figure 12S: Temperature dependent fluorescence spectra of the ligand, **L.** Fluorescence intensity increases with increasing temperature (30°C to 100°C, 0.1mM solution in DMF, λ_{ex} = 340 nm)

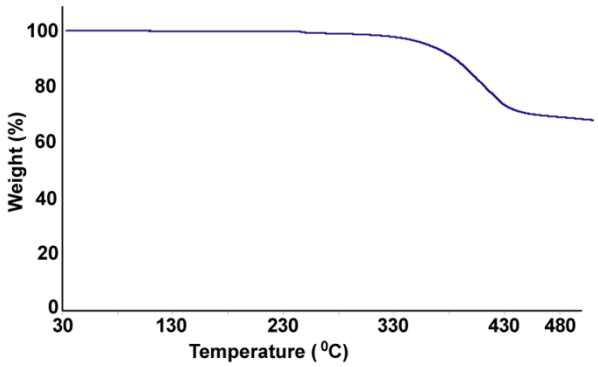


Figure 13S: Thermogravimetry of the complex **1**

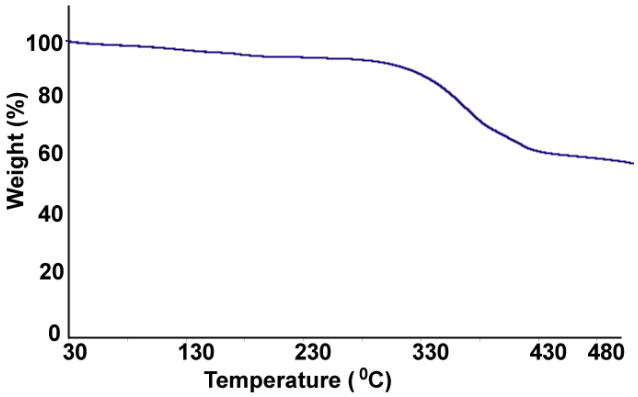


Figure 14S: Thermogravimetry of the complex **2**. In case of the complex**2**, the decomposition of the organic ligand started from 280 °C

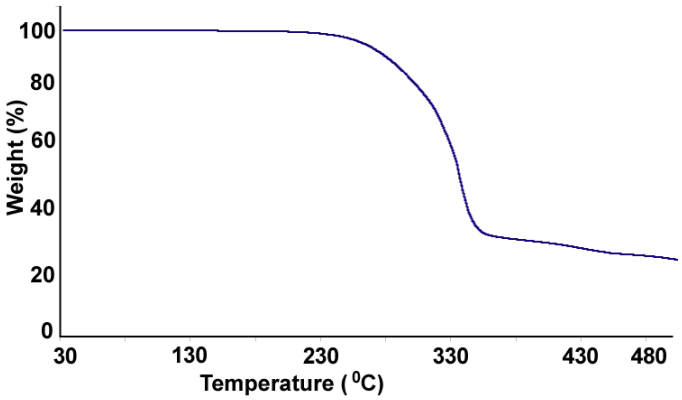


Figure 15S: Thermogravimetry of the complex **3**

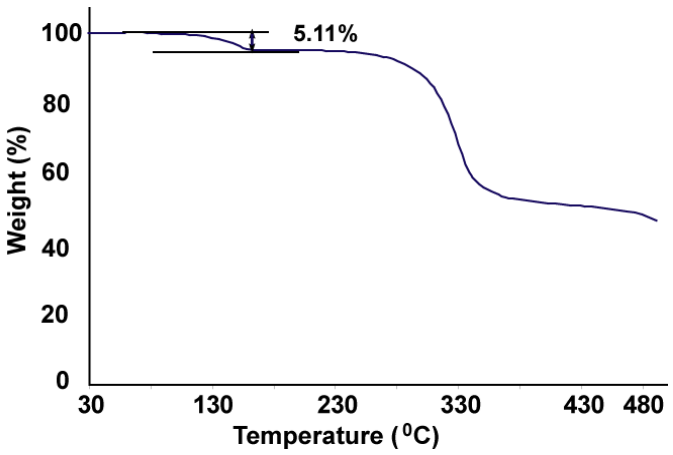


Figure 16S: Thermogravimetry of the complex **4** (For the complex **4**, one step weight loss due to the two solvent acetonitrile molecules takes place in the temperature range 70−170 °C corresponding to a weight loss of 5.11% (calcd 5.56%). The decomposition of ligand at 250 °C-460 °C.

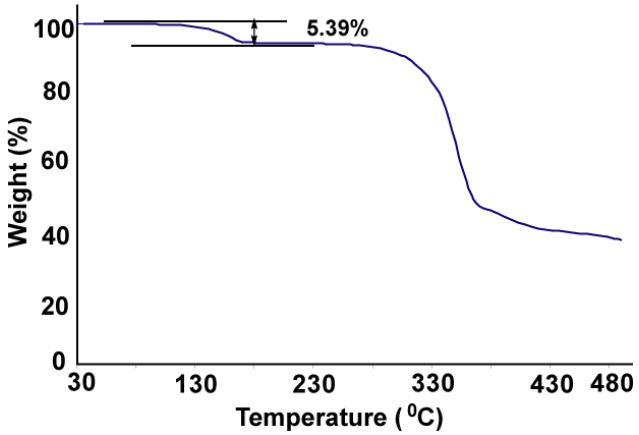


Figure 17S: Thermogravimetry of the complex **5.** The two solvent acetonitrile molecules are lost in the range 88-200 °C corresponding to a weight loss of 5.39 % (calcd. 5.55 %) and the decomposition of organic ligands at 260 °C-460 °C.

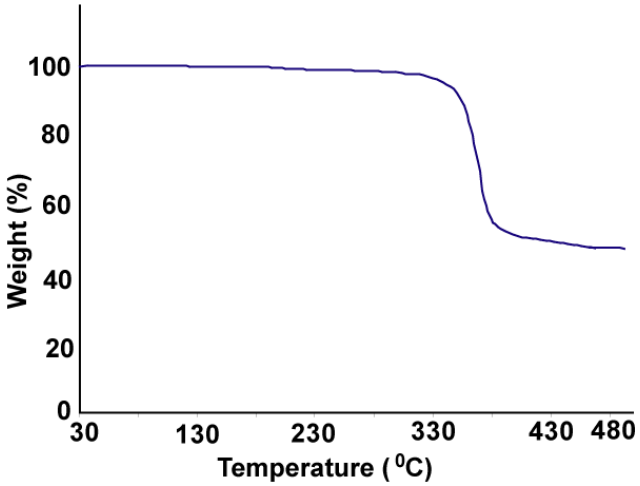


Figure 18S: Thermogravimetry of the complex **6.** Complex **6** shows a gradual one step weight loss due to the degradation of organic ligands in the temperature range 130-460 °C.

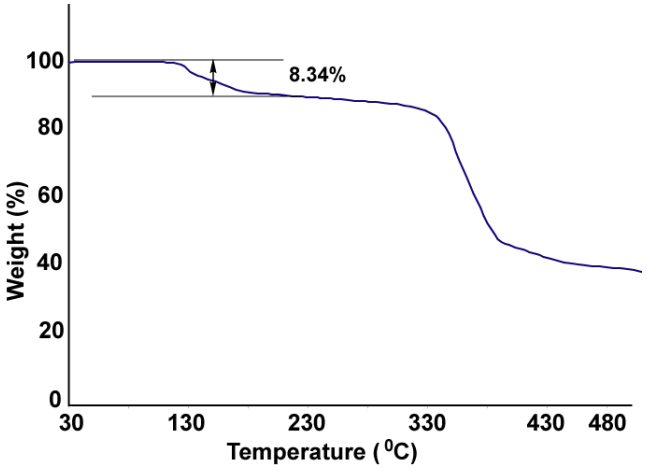
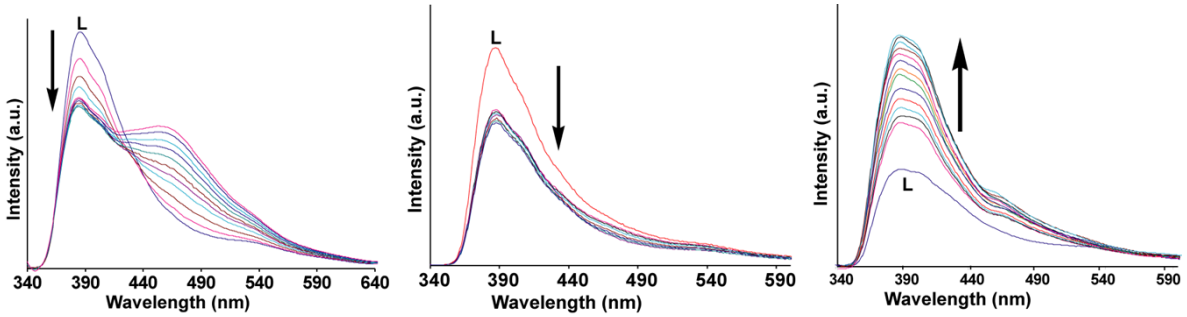


Figure 19S: Thermogravimetry of the complex **7.** The complex **7** shows weight loss of 8.34 wt % (calcd. 8.98 wt%) in the range of 120-182 °C corresponds to the loss of one lattice dimethylformamide molecule and one coordinated dimethylformamide molecule.



(a) (b) (c)

Figure 20S: The changes in the intensity of fluorescence emission (λ_{ex} = 340nm) of the ligand, **L** (2ml of 10^{-4} M solution in DMF) on addition of (a) $ZnCl_2$, (b) $CdCl_2$ and (c) $HgCl_2$ (5µl aliquots of 10^{-2} M solution in methanol**) .**

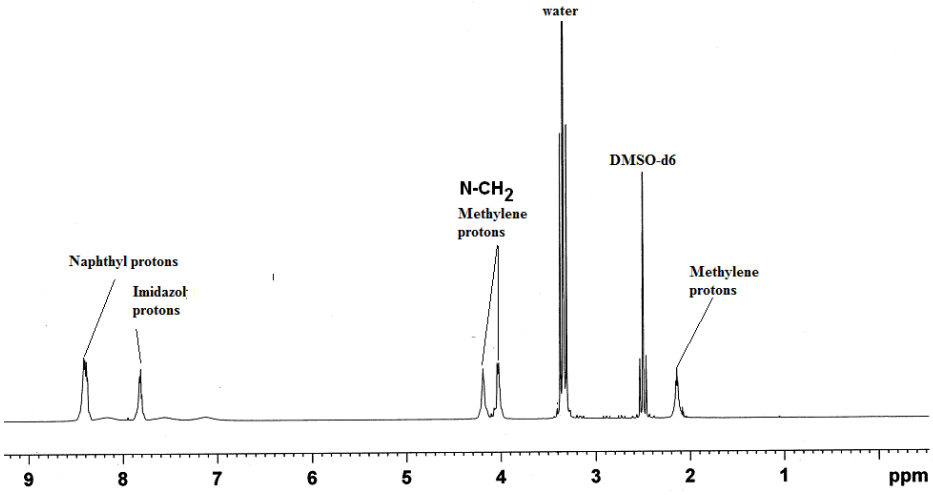


Figure 21S: ^{1}H-NMR (600 MHz, DMSO-d_6) spectra of the complex **6.**

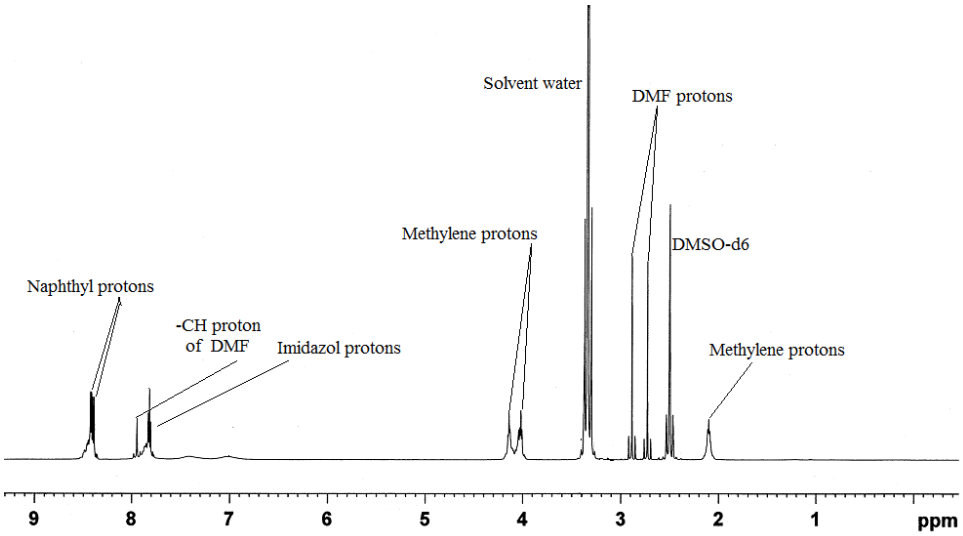


Figure 22S: ^{1}H-NMR (600 MHz, DMSO-d_6) spectra of the complex **7.**