Supplementary Information

Table S1 Selected bond lengths (Å) and bond angles (°) of Ni(II) and Co(II) centers in the compounds **1**and **2** respectively.

Bond distances of 1 (in Å)		Bond angles of 1 (in Degree)	
Mn1–Cl1	2.4485(11)	N1A–Mn1–N1B	152.42(12)
Mn1–Cl2	2.4424(11)	N1A–Mn1–N10B	90.11(12)
Mn1–N1A	2.261(4)	N1B–Mn1–N10B	72.12(12)
Mn1–N10A	2.343(4)	NA–Mn1–N10A	71.99(13)
Mn1–N1B	2.284(3)	N1B–Mn1–N10A	85.34(12)
Mn1–N10B	2.320(3)	N10B–Mn1–N10A	85.22(12)
		N10A–Mn1–Cl1	104.06(9)
		N1A–Mn1–Cl2	92.28(8)
		N1B–Mn1–Cl2	164.38(9)
		N10B–Mn1–Cl2	92.87(9)
		N10A–Mn1–Cl2	94.5(1)
		N1A–Mn1–Cl1	105.22(9)
		N10B–Mn1–Cl1	87.27(9)
		N10A–Mn1–Cl1	164.49(9)
		Cl2–Mn1–Cl1	97.94(4)
Bond distances of 2 (in Å)		Bond angles of 2 (in Degree)	
Zn1–O3	2.016(2)	O3–Zn1–N1	106.26(9)
Zn1–N1	2.070(3)	O3–Zn1–N3	96.24(9)
Zn1–N3	2.071(2)	N1–Zn1–N3	104.32(10)
Zn1–O1	2.105(3)	O3–Zn1–O2	92.21(9)
Zn1–O2	2.292(3)	N1–Zn1–O2	143.86(11)
Zn1–C1	2.535(3)	N3–Zn1–O2	104.17(9)
		O1–Zn1–O2	59.39(10)
		O3–Zn1–O1	149.88(11)
		N1–Zn1–O1	93.92(10)
		N3–Zn1–O1	100.20(11)

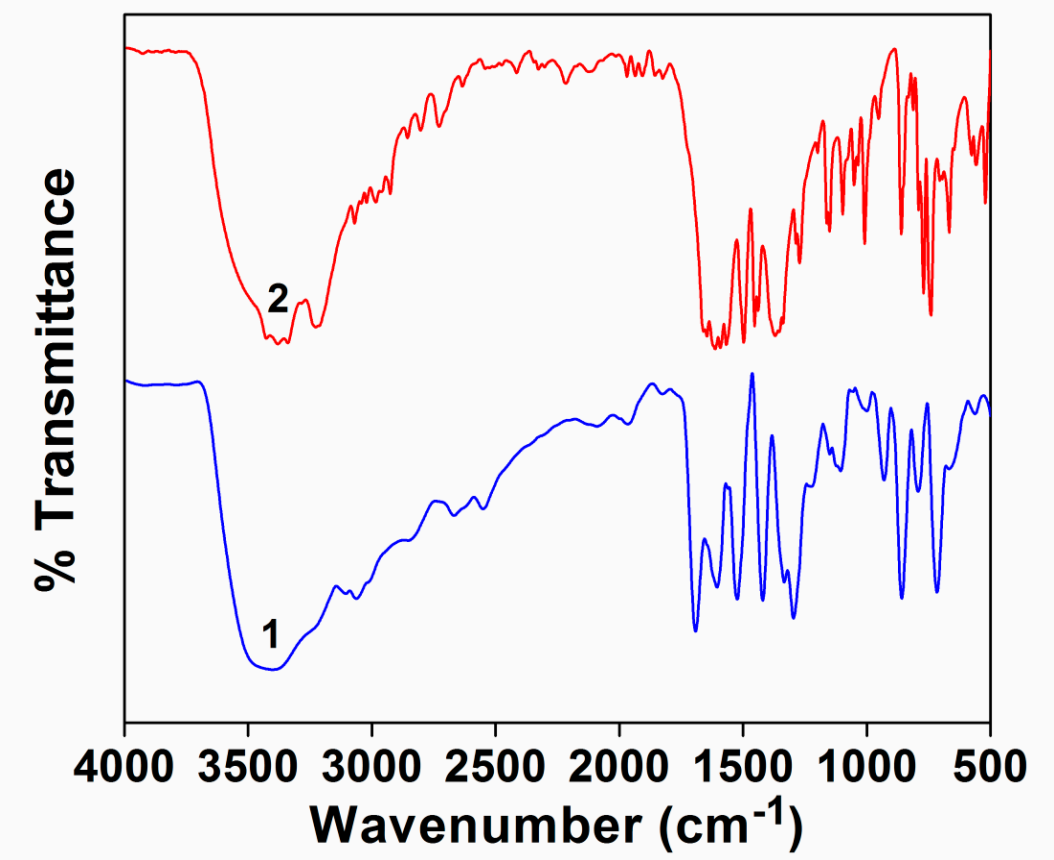
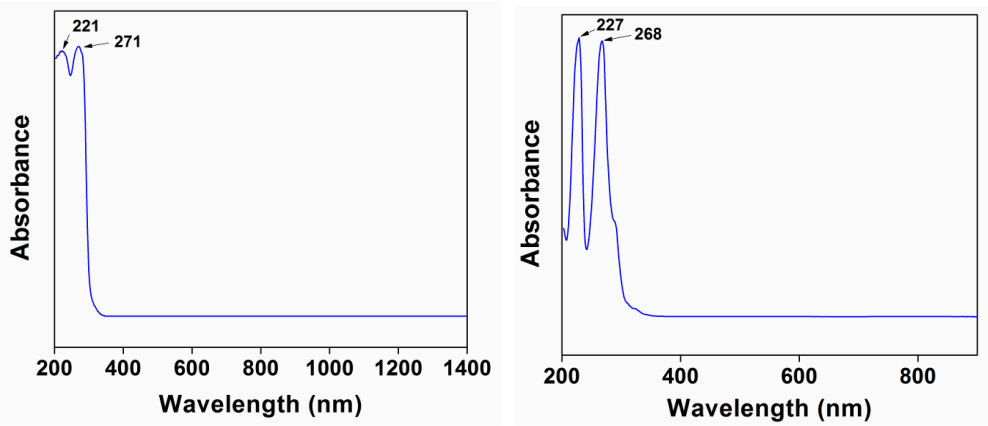


Figure S1. FT-IR Spectra of compounds **1** and **2**.

2.3.2 Electronic spectroscopy

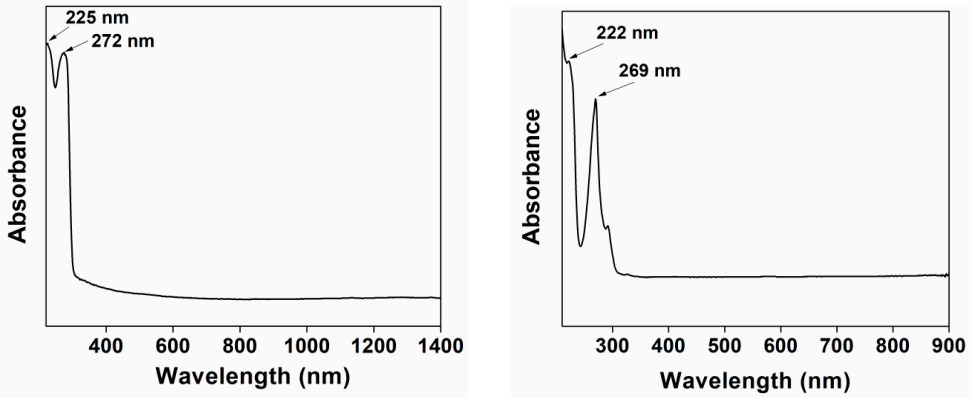
The electronic spectra of the compounds **1** and **2** have been recorded in solid as well as in aqueous state (Figure S2-S3). The electronic spectra of compound **1** does not exhibit any absorption bands in the visible region, as Mn(II) centre (d^5 system) has all the electronic transitions from the $^6A_{1g}$ ground state doubly forbidden [1-2]. The peaks at 221 and 271 nm in the solid state UV-Vis-NIR spectrum can be assigned to the π→π* transition of the aromatic ligand [3]. In the aqueous state UV-Vis spectrum these absorption peaks were obtained at 227 and 268 nm respectively [3].



(**a**) (**b**)

Figure S2. (**a**) UV-Vis-NIR spectrum of **1** (**b**) UV-Vis spectrum of compound **1**

The electronic spectra of the diamagnetic Zn(II) compound (**2**) do not show any absorption bands (Figure S3) in the visible region [4-6]. The absorption bands at 225 and 272 nm in the UV-Vis-NIR spectrum of compound **2** can be attributed to the π→π* transition of the aromatic ligands [7]. These absorption peaks are obtained at 222 and 269 nm in the aqueous phase UV-Vis spectrum. The observed similarities in the absorption peaks of compounds **1** and **2** in both the phases suggest that the compounds do not undergo any structural distortion in the aqueous phase [8,9].



(**a**) (**b**)

Figure S3. (**a**) UV-Vis-NIR spectrum of **2** (**b**) UV-Vis spectra of compound **2**

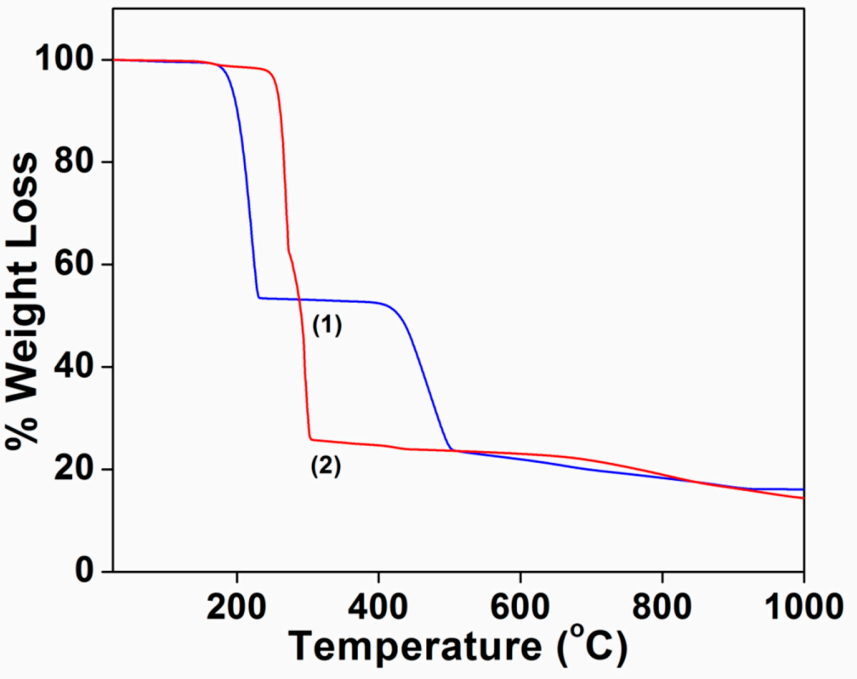


Figure S4. TG analysis of compounds **1** and **2**.

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