

Supplementary Information

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

Bond lengths of 1 (in Å)		Bond angles of 1 (in Degree)	
Ni1–O3	2.063(2)	O3–Ni1–O4	87.74(9)
Ni1–O4	2.067(2)	O3–Ni1–N2	173.84(10)
Ni1–N2	2.069(3)	O4–Ni1–N2	90.20(11)
Ni1–O1	2.074(2)	O3–Ni1–O1	91.46(9)
Ni1–N1	2.078(3)	O4–Ni1–O1	88.65(9)
Ni1–O2	2.108(2)	N2–Ni1–O1	94.29(10)
Ni2–N3	2.086(3)	O3–Ni1–N1	89.95(11)
Ni2–N4	2.113(3)	O4–Ni1–N1	94.35(10)
Ni2–O5	2.131(2)	N2–Ni1–N1	84.42(12)
Ni3–N6	1.962(2)	O1–Ni1–N1	176.74(10)
Ni3–N5	1.976(3)	O3–Ni1–O2	88.10(9)
Ni3–O10	2.094(2)	O4–Ni1–O2	172.99(9)
Ni3–O11	2.124(2)	N2–Ni1–O2	94.49(10)
Ni3–O6	2.139(2)	O1–Ni1–O2	85.82(8)
Ni3–O8	2.156(2)	N1–Ni1–O2	91.29(9)
Ni4–N7	1.968(2)	N3–Ni2–N3#	180.0
Ni4–N8	1.972(2)	N3–Ni2–N4#	96.88(10)
Ni4–O16	2.104(2)	N3–Ni2–N4	83.12(10)
Ni4–O18	2.126(2)	N4–Ni2–N4#	180.0
Ni4–O14	2.134(2)	N3–Ni2–O5	90.67(10)
Ni4–O20	2.135(2)	N3–Ni2–O5#	89.33(10)
Ni5–N9	2.101(3)	N4–Ni2–O5	87.53(9)
Ni5–N10	2.100(3)	N4–Ni2–O5#	92.47(9)
Ni5–O26	2.113(2)	N4#–Ni2–O5	92.47(9)
		O5–Ni2–O5#	180.0
		N6–Ni3–N5	175.11(11)
		N6–Ni3–O10	78.47(9)
		N5–Ni3–O10	106.41(9)
		N6–Ni3–O11	78.10(9)
		N5–Ni3–O11	97.02(9)
		O10–Ni3–O11	156.55(8)
		N6–Ni3–O6	101.00(9)
		N5–Ni3–O6	77.94(9)
		O10–Ni3–O6	95.35(8)
		O11–Ni3–O6	90.49(9)
		N6–Ni3–O8	102.59(9)
		N5–Ni3–O8	77.46(9)
		O10–Ni3–O8	90.74(8)
		O11–Ni3–O8	93.33(8)
		O6–Ni3–O8	155.39(8)
		N7–Ni4–N8	178.11(11)
		N7–Ni4–O16	79.04(9)

		N8–Ni4–O16	102.74(9)
		N7–Ni4–N18	102.54(9)
		N8–Ni4–N18	78.13(9)
		O16–Ni4–O18	91.13(9)
		N7–Ni4–O14	77.54(9)
		N8–Ni4–O14	100.67(9)
		O16–Ni4–O14	156.54(8)
		O18–Ni4–O14	95.27(8)
		N7–Ni4–O20	101.60(9)
		N8–Ni4–O20	77.70(9)
		O16–Ni4–O20	94.64(9)
		O18–Ni4–O20	155.83(8)
		O14–Ni4–O20	88.71(8)
		N9–Ni5–N9#	180.0
		N9#–Ni5–N10#	96.31(11)
		N9–Ni5–N10	96.31(11)
		N9#–Ni5–N10	83.69(11)
		N10–Ni5–N10#	180.0
		N9–Ni5–O26#	91.12(10)
		N9#–Ni5–O26#	88.88(10)
		N10–Ni5–O26#	84.51(10)
		N10–Ni5–O26	95.49(10)
		O26–Ni5–O26#	180.0
Bond lengths of 2 (in Å)		Bond angles of 2 (in Degree)	
Zn1–N1	2.013(2)	N1–Zn1–N1#1	105.11(1)
Zn1–N1#1	2.013(2)	N1–Zn1–N12	127.44(6)
Zn1–N12	2.019(3)	N1#1–Zn1–N12	127.44(6)
Zn1–O8	2.154(2)	N1–Zn1–O8#1	104.65(8)
Zn1–O8#1	2.154(2)	N1–Zn1–O8	91.62(8)
		N12–Zn1–O8	76.63(5)
		N1#1–Zn1–O8#1	91.62(8)

#1 1-X, +Y, 1/2-Z

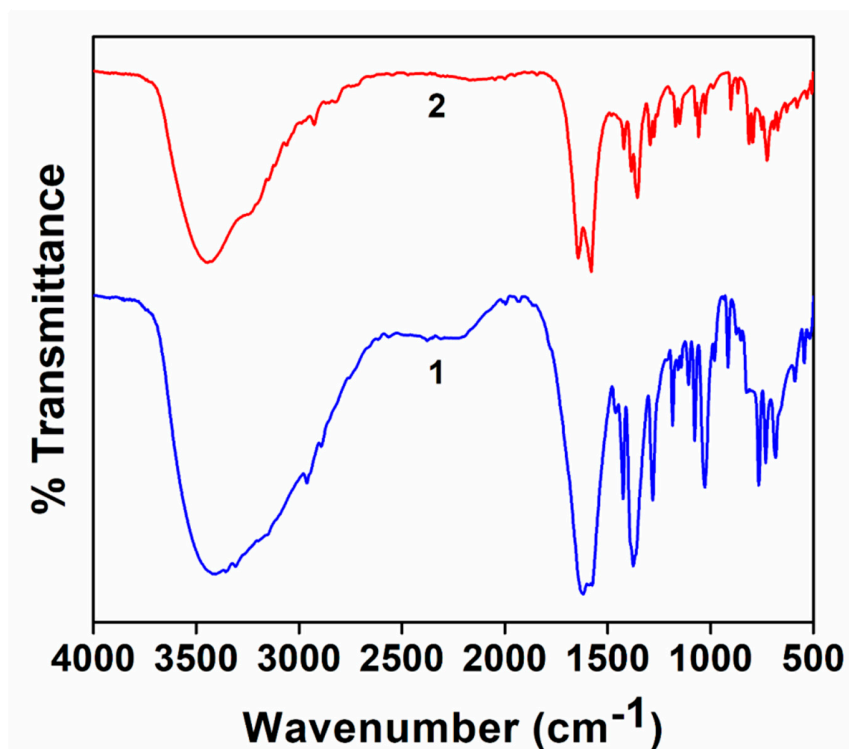


Figure S1. FT-IR Spectra of compounds **1** and **2**.

2.3.2 Electronic Spectroscopy

The electronic spectra of the compounds **1** and **2** have been determined in both solid and aqueous phases (Figures S2a and S2b). Three ligand field bands at 1060, 612 and 366 nm are observed in the solid phase UV-Vis-NIR spectrum of **1** (Figure S2a) which can be attributed to the spin allowed transitions from the ground to the excited triplet states *viz.*; $[^3A_{2g} \rightarrow ^3T_{2g}(F)](v_1)$, $[^3A_{2g} \rightarrow ^3T_{1g}(F)](v_2)$ and $[^3A_{2g} \rightarrow ^3T_{1g}(P)](v_3)$, respectively [1,2]. The absorption bands due to $\pi \rightarrow \pi^*$ transition is obtained at 271 nm [3]. In the aqueous phase UV-Vis spectrum (Figure S2b) of **1**, the band corresponding to $\pi \rightarrow \pi^*$ transition of the aromatic ligands is appeared at 267 nm [3]. The absorption bands at 589 nm and at 364 nm in the UV-Vis spectrum of **1** can be assigned to

${}^3A_{2g}(F) \rightarrow {}^3T_{1g}(F)$ and ${}^3A_{2g}(F) \rightarrow {}^3T_{1g}(P)$ transitions respectively for octahedral Ni(II) ions [4]. The NIR band cannot be visualized in the solution spectrum due to the limitation in the wavelength window of the spectrophotometer utilized for this purpose [5].

The spectra of **2** do not show spectral band in the visible region which can be attributed to the d^{10} electronic configuration of the Zn(II) centers that does not allow any electronic transition to the higher excited electronic states [6,7]. The absorption peaks at 229, 269 nm in UV-Vis-NIR (Figure S3a) and 221 nm, 264 nm in UV-Vis spectrum (Figure S3b) can be attributed to the $\pi \rightarrow \pi^*$ transitions of aromatic ligands [3,8]. The marked resemblance in the absorption bands in both the phases of the spectra of compounds **1** and **2** reflects the similarities in bonding modes and the geometries of the compounds in both the phases [9,10].

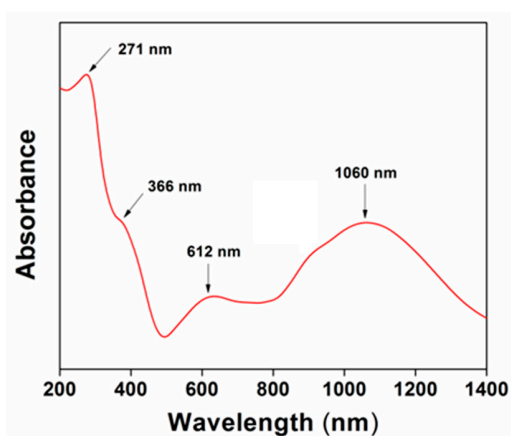
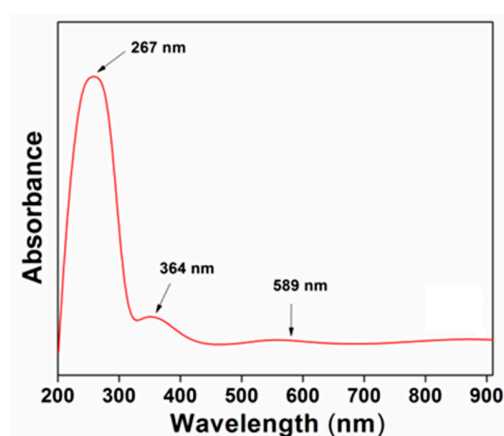


Figure S2. (a) UV-Vis-NIR spectrum of **1**



(b) UV-Vis spectrum of **1**

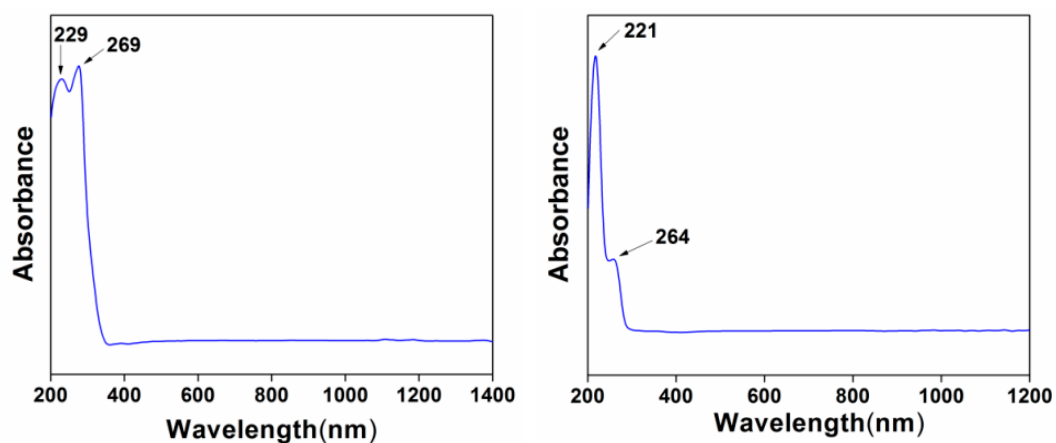


Figure S3. (a) UV-Vis-NIR spectrum of 2

b) UV-Vis spectrum of 2

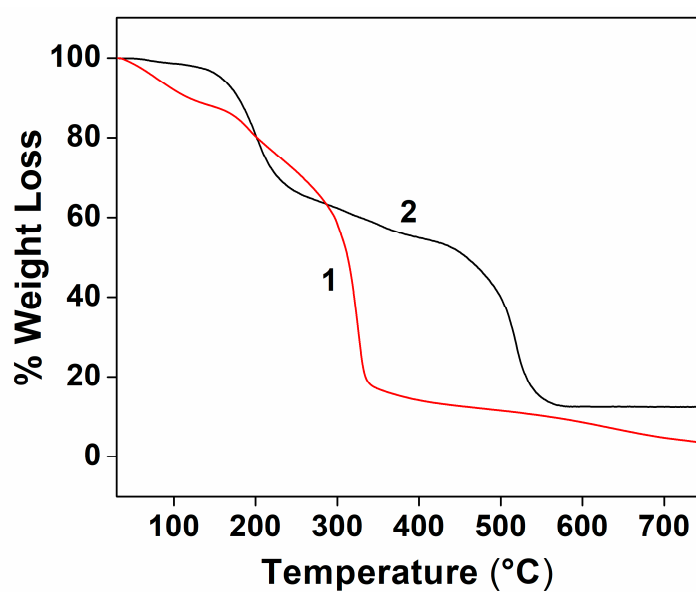


Figure S4. Thermogravimetric curves of the compounds 1 and 2.

Supplementary references

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