Supplementary Information

3.2. IR spectra

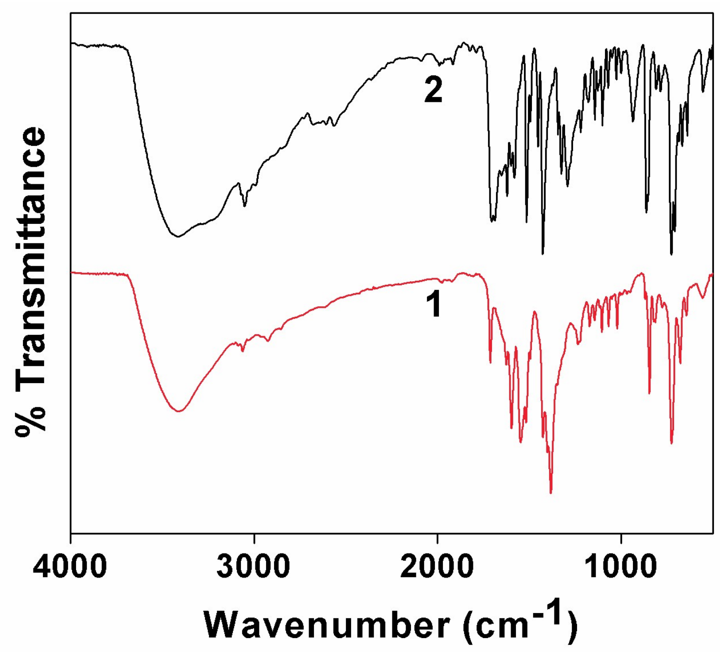
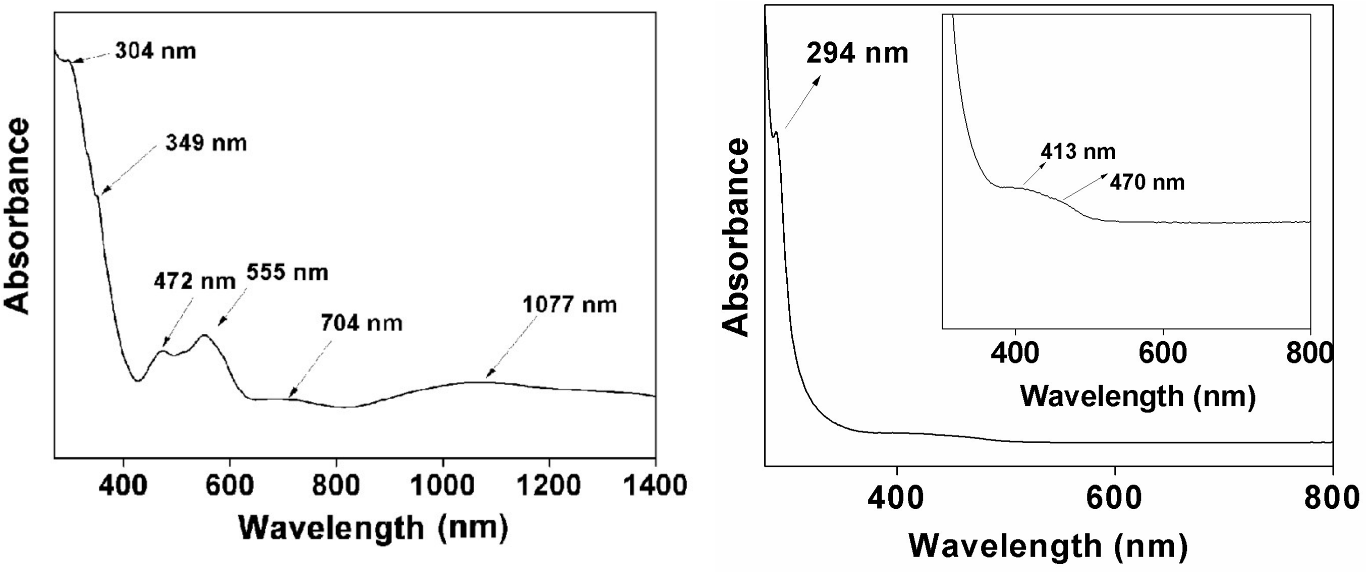


Fig. S1 FT-IR spectra of compounds **1** and **2**

FT-IR spectra of the synthesized compounds have been recorded in the region 4000–500 cm^{-1} [Fig. S1]. The coordination of *phen* to the Co(II) and Zn(II) metal centers in complexes **1** and **2** are indicated by the shifting of IR frequencies for δ(C–H) vibrations of *phen.*[41] The bands in the range 3421-3370 cm^{-1} for both the complexes could be assigned to the stretching vibration of the water involving hydrogen bonding.[42] The IR spectral bands within 1300-1650 cm^{-1} region are difficult to assign due to the appearance of several absorption bands both for the *phen* and bz ligands of the complexes.[43] A strong absorption band at 1539 cm^{-1} indicates the presence of aromatic bzH in the lattice of compound **2**.[44] The difference between the asymmetric stretching, $\nu_{as}(COO^-)$ and symmetric stretching vibration bands, $\nu_s(COO^-)$ for compound **1** is observed below 200 cm^{-1} which indicates monodentate binding of bz at Co(II) metal centre.[45]

3.3 Electronic spectra

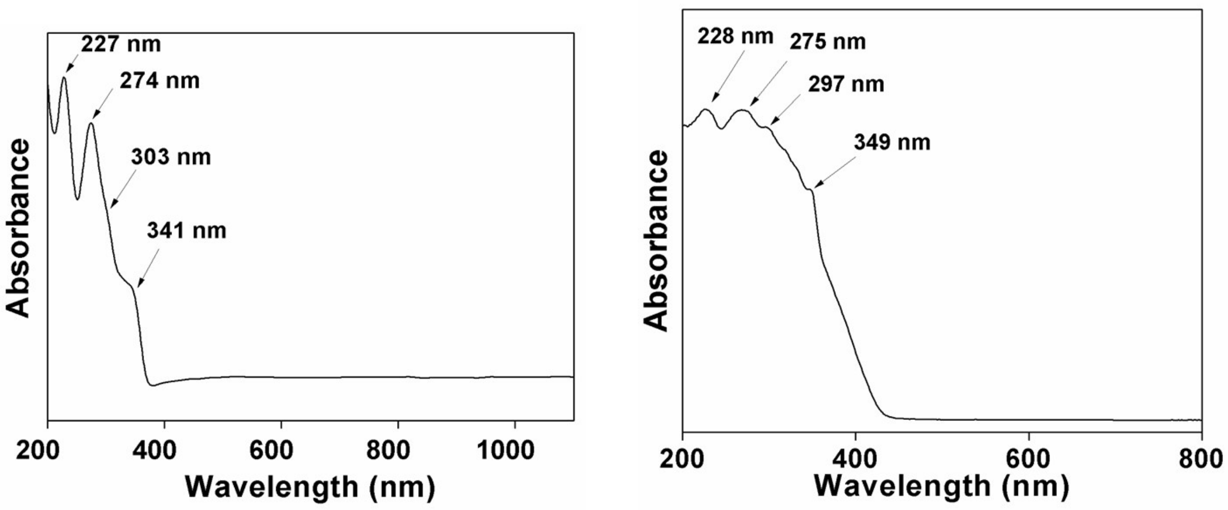


(**a**) (**b**)

Fig. S2 (a) Solid state UV-vis-NIR spectrum of **1** (b) UV-vis spectrum of **1** in water (10^{-3}M)

Solid state UV-Vis-NIR spectrum of complex **1** exhibit bands at 304 nm and 349 nm assigned to $\pi\rightarrow\pi^*$ and n $\rightarrow\pi^*$ transitions of the aromatic ligand [Fig. S2(a)]. Three ligand field bands viz. $^4T_{1g}(F)\rightarrow{}^4T_{2g}(F)$ (ν_1), $^4T_{1g}(F)\rightarrow{}^4A_{2g}(F)$ (ν_2) and $^4T_{1g}(F)\rightarrow{}^4T_{1g}(P)$ (ν_3) for high-spin octahedral Co(II) complex for **1** is observed in solid state spectrum.[46] The first band occurs at 1077 nm, the third band is seen at 472 nm, and the ν_2 band due to $^4T_{1g}(F)\rightarrow{}^4A_{2g}(F)$ appears at 555 nm. The extra band at 704 nm appeared for ν_2 can be attributed either to spin orbit coupling or to transition to doublet state.[46] However, the spectrum in water [Fig. S2(b)] shows weak absorption bands at 413 nm and 470 nm assigned to $^4T_{1g}(F)\rightarrow{}^4T_{1g}(P)$ (ν_3) and $^4T_{1g}(F)\rightarrow{}^4A_{2g}(F)$ (ν_2) transitions. The NIR band is not seen in the solution spectrum because of the limit in wavelength window of the spectrophotometer used.[47]

The electronic spectra of compound **2** are shown in Fig. S3. Compound **2** shows no spectral band in the visible region in both aqueous and solid phases, which can be attributed to the d^{10} configuration of the Zn(II) centre that does not allow any electronic transition to the higher excited electronic states.[48] Characteristic absorptions in the solid and aqueous phase in the wavelength range 227–275 nm for compound **2** is observed due to π–π* and n–π* transitions of the aromatic ring of *phen* and bz moiety. In the wavelength range 297-349 nm, the absorption bands are observed due to ligand to metal charge transfer transitions.[49-50]



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

Fig. S3 (a) Solid state UV-vis-NIR spectrum of **2** (b) UV-vis spectrum of **2** in water (10^{-3}M)