3.2 Infrared Spectroscopy

FT-IR spectra of the compounds 1 and 2 (KBr phase) were recorded in the region 3500–400 cm\(^{-1}\) (Fig. S1). For complexes 1 and 2, strong absorption bands appearing at 1602 cm\(^{-1}\) and 1607 cm\(^{-1}\) respectively for the asymmetric stretching and 1385 cm\(^{-1}\) and 1398 cm\(^{-1}\) respectively for the symmetric stretching of the carboxylate groups. The difference between the asymmetric and symmetric stretching vibrations for 1 and 2 are 217 cm\(^{-1}\) and 209 cm\(^{-1}\) respectively which suggest that benzoate ligand behaves as a bi-chelating oxygen donor ligand in 1 and bidentate ligand in 2 at the metal centers. The bands in the region of 3420‒3450 cm\(^{-1}\) for both the complexes 1 and 2 could be assigned to the stretching vibration of the water involving hydrogen bonding.\(^{48}\) The ring stretching vibrations [\(\nu(C=C)\) and \(\nu(C=N)\)] of phenanthroline moiety for both the compounds observed in expected positions. The IR frequencies for \(\delta(C–H)\) vibrations of phen in 1 and 2 respectively around 720 and 633 cm\(^{-1}\) are shifted to around 840 cm\(^{-1}\) and 799 cm\(^{-1}\) suggesting the coordination of phenanthroline to the Cu(II) metal centers. The strong absorption bands at 1386 cm\(^{-1}\) suggest the presence of free nitrate in 1.\(^{49}\)
3.3 Electronic spectra of 1 and 2

![UV-Vis spectra of 1 and 2](a)

![UV-Vis-NIR spectra of 1 and 2](b)

**Fig. S2** (a) UV-Vis spectra of 1 and 2 in aqueous phase (b) UV-Vis-NIR spectra of 1 and 2 in solid phase

We have recorded the UV-Vis spectra of both the complexes 1 and 2, in solid state as well as in solution. In the UV–Vis absorption spectra of 1 and 2, the sharp and intense absorption band around 346 nm corresponds to the ligand to metal charge transfer transition (**Fig. S2a**). However, the presence of broad absorption band for 1 around 631 nm is due to the distortion of the compound around the Cu(II) centers in the aqueous phase. In complex 2, a broad visible absorption band at 638 nm may be attributed to the $^2E_g \rightarrow ^2T_{2g}$ transition for octahedral complexes. The UV-Vis-NIR spectrum of compound 1 (**Fig S2b**) shows a broad asymmetric band (644 nm) with expected splitting for the local C$_{4v}$ symmetry of the Cu(II) centers in the square pyramidal geometry. The UV-Vis-NIR spectrum of 2 (**Fig. S2b**) shows broad absorption at 629 nm which may be thought to result from the splitting of the usual $^2E_g \rightarrow ^2T_{2g}$ transition for octahedral complexes. The UV bands originating from the ligand to metal charge transfer transition found in the expected positions for both the complexes.