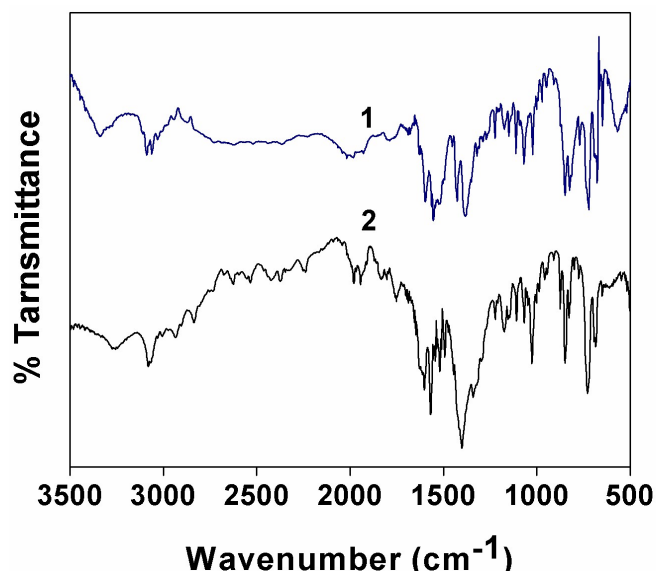


1 **Supplementary Information**

2 **3.2 Infrared Spectroscopy**



5 **Fig. S1** FTIR spectra of **1** and **2** in KBr phase

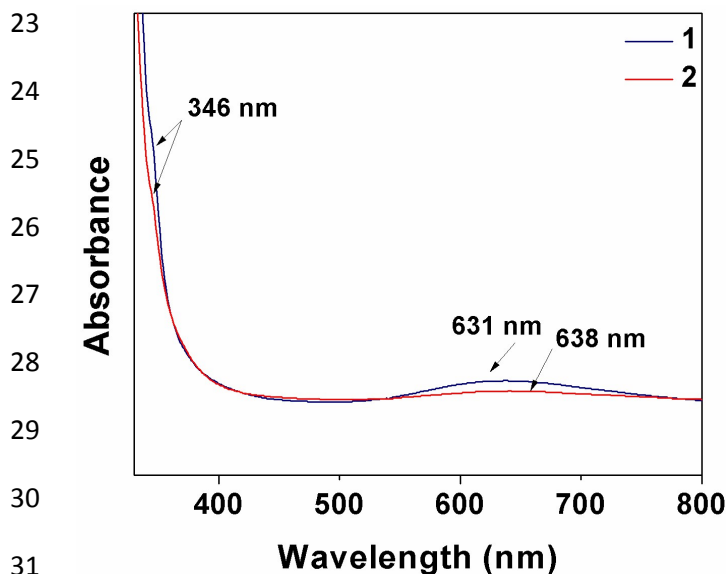
6

7 FT-IR spectra of the compounds **1** and **2** (KBr phase) were recorded in the region 3500–
8 400 cm^{-1} (**Fig. S1**). For complexes **1** and **2**, strong absorption bands appearing at 1602 cm^{-1} and
9 1607 cm^{-1} respectively for the asymmetric stretching and 1385 cm^{-1} and 1398 cm^{-1} respectively
10 for the symmetric stretching of the carboxylate groups. The difference between the asymmetric
11 and symmetric stretching vibrations for **1** and **2** are 217 cm^{-1} and 209 cm^{-1} respectively which
12 suggest that benzoate ligand behaves as a bi-chelating oxygen donor⁴⁷ ligand in **1** and bidentate
13 ligand in **2** at the metal centers. The bands in the region of 3420–3450 cm^{-1} for both the
14 complexes **1** and **2** could be assigned to the stretching vibration of the water involving hydrogen
15 bonding.⁴⁸ The ring stretching vibrations [$\nu(\text{C}=\text{C})$ and $\nu(\text{C}=\text{N})$] of phenanthroline moiety for both
16 the compounds observed in expected positions. The IR frequencies for $\delta(\text{C}-\text{H})$ vibrations of
17 phen in **1** and **2** respectively around 720 and 633 cm^{-1} are shifted to around 840 cm^{-1} and 799 cm^{-1}
18 suggesting the coordination of phenanthroline to the Cu(II) metal centers. The strong
19 absorption bands at 1386 cm^{-1} suggest the presence of free nitrate in **1**.⁴⁹

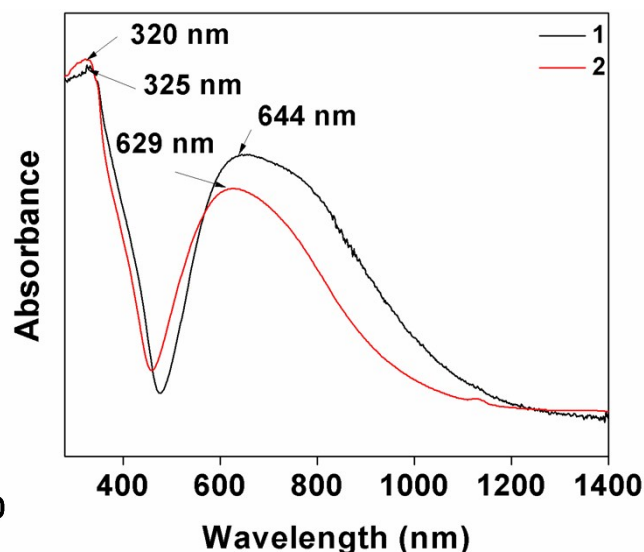
20

21 3.3 Electronic spectra of 1 and 2

22



(a)



(b)

34 **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

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36

37 We have recorded the UV-Vis spectra of both the complexes **1** and **2**, in solid state as

38 well as in solution. In the UV-Vis absorption spectra of **1** and **2**, the sharp and intense absorption

39 band around 346 nm corresponds to the ligand to metal charge transfer transition (**Fig. S2a**).

40 However, the presence of broad absorption band for **1** around 631 nm is due to the distortion of

41 the compound around the Cu(II) centers in the aqueous phase. In complex **2**, a broad visible

42 absorption band at 638 nm may be attributed to the ${}^2E_g \rightarrow {}^2T_{2g}$ transition for octahedral

43 complexes.⁵⁰ The UV-Vis-NIR spectrum of compound **1** (**Fig S2b**) shows a broad asymmetric

44 band (644 nm) with expected splitting for the local C_{4v} symmetry of the Cu(II) centers in the

45 square pyramidal geometry. The UV-Vis-NIR spectrum of **2** (**Fig. S2b**) shows broad absorption

46 at 629 nm which may be thought to result from the splitting of the usual ${}^2E_g \rightarrow {}^2T_{2g}$ transition for

47 octahedral complexes.⁵¹ The UV bands originating from the ligand to metal charge transfer

48 transition found in the expected positions for both the complexes.⁵²

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