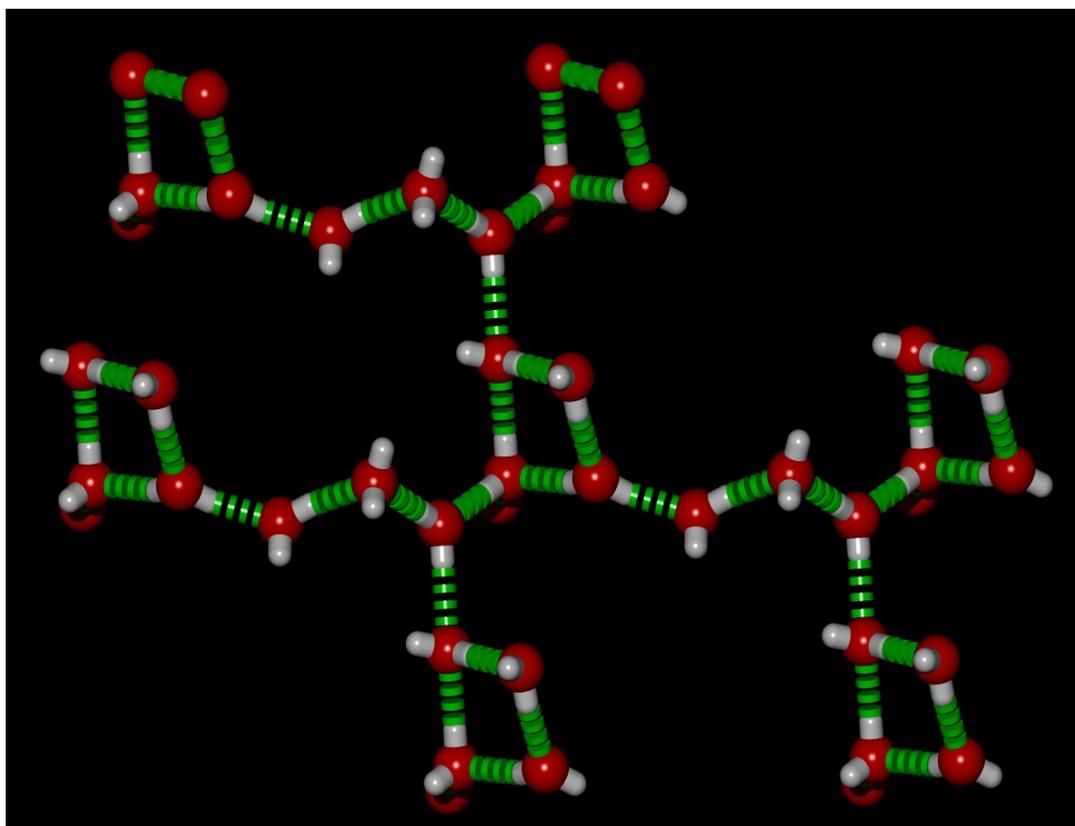
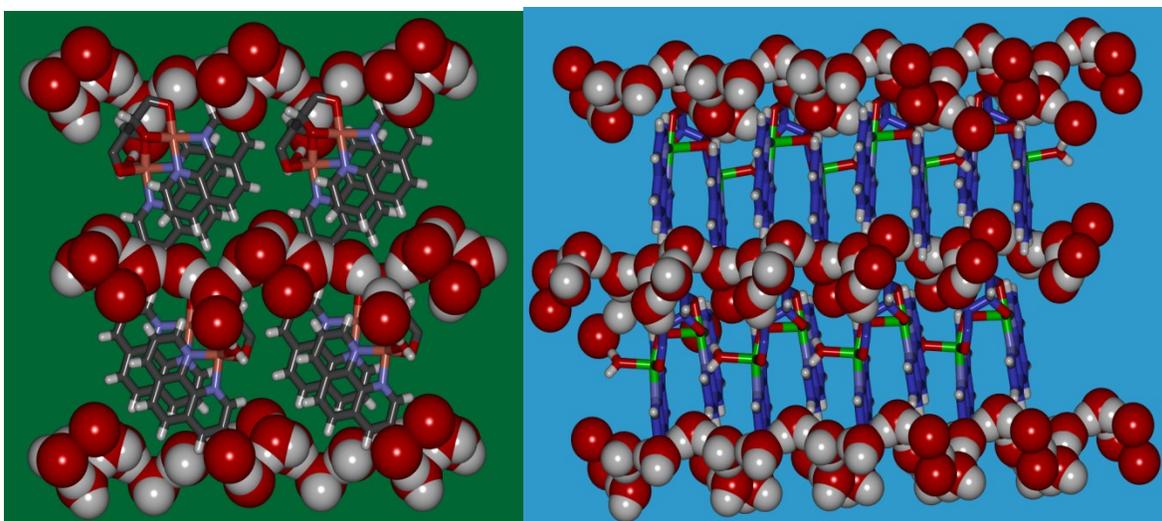


# pH-triggered construction of NLO active CMOFs: change in supramolecular assembly, water clusters, helical architectures and their properties

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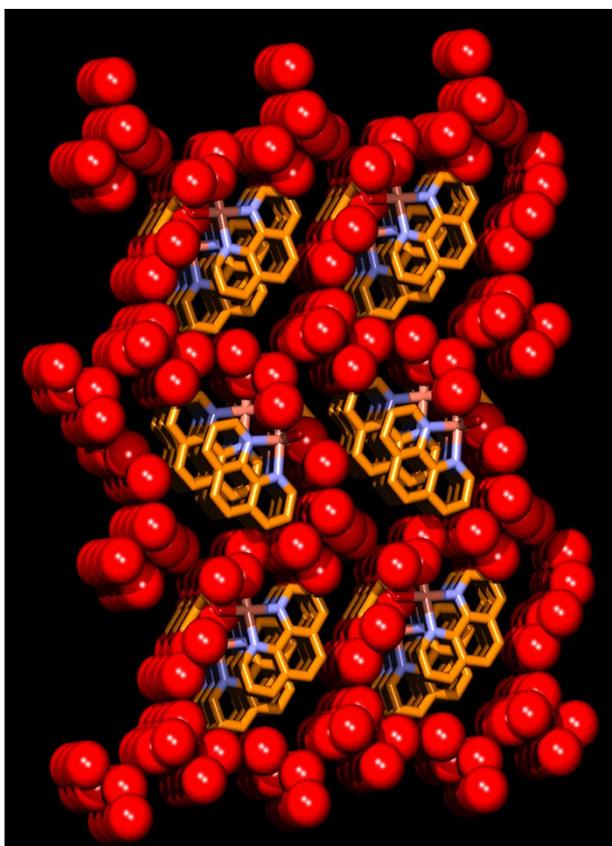
**Figure S1:** Each water tetramers are connected by six other tetramers by hydrogen bonding in complex **1** (O=Red and H=Hydrogen)



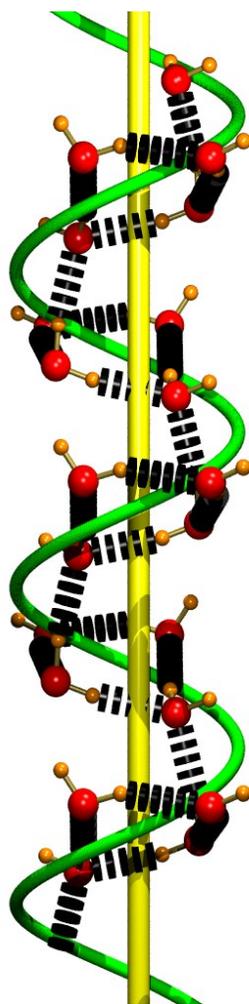
(a) along  $bc$ -plane

(b) along  $a$ -axis

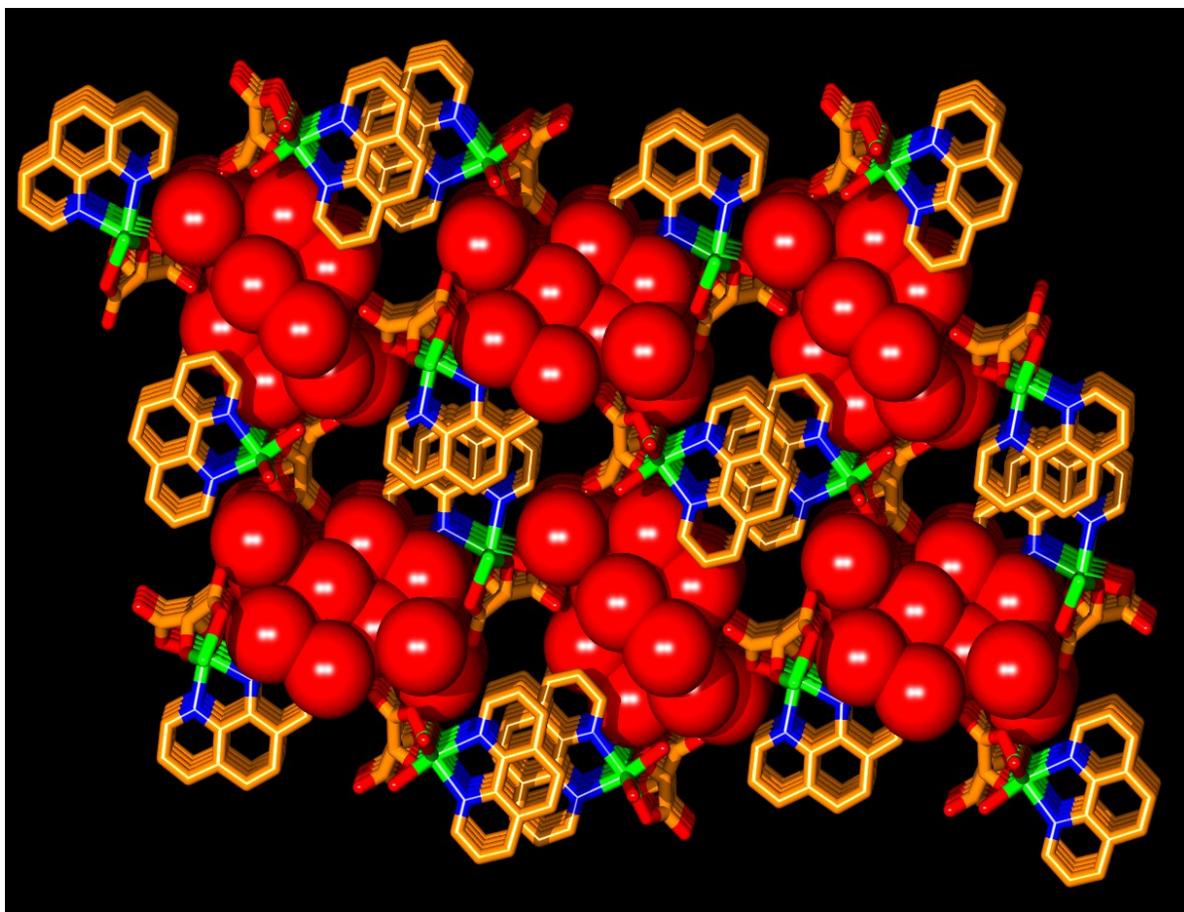
**Figure S2:** The supramolecular chains are in between two parallel water sheets (C=Grey(a); Deep Blue(b), O=Red, H=White)



**Figure S3:** The 3D metallosupramolecular network of complex **1**



**Figure S4:** The 1D helical water chains in complex 2 (O=Red and H=Orange)



**Figure S5:** The 3D metallosupramolecular network of complex **2**

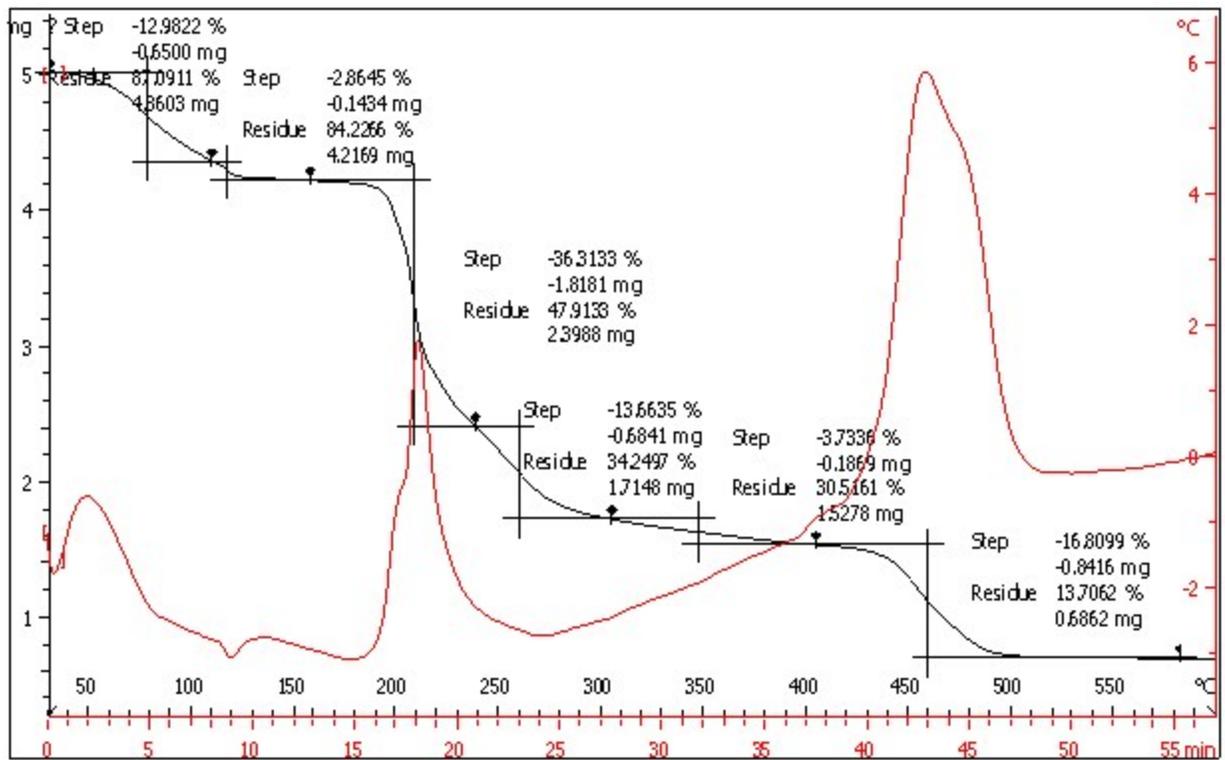


Figure S6: The TG-DTA curve of complex 1

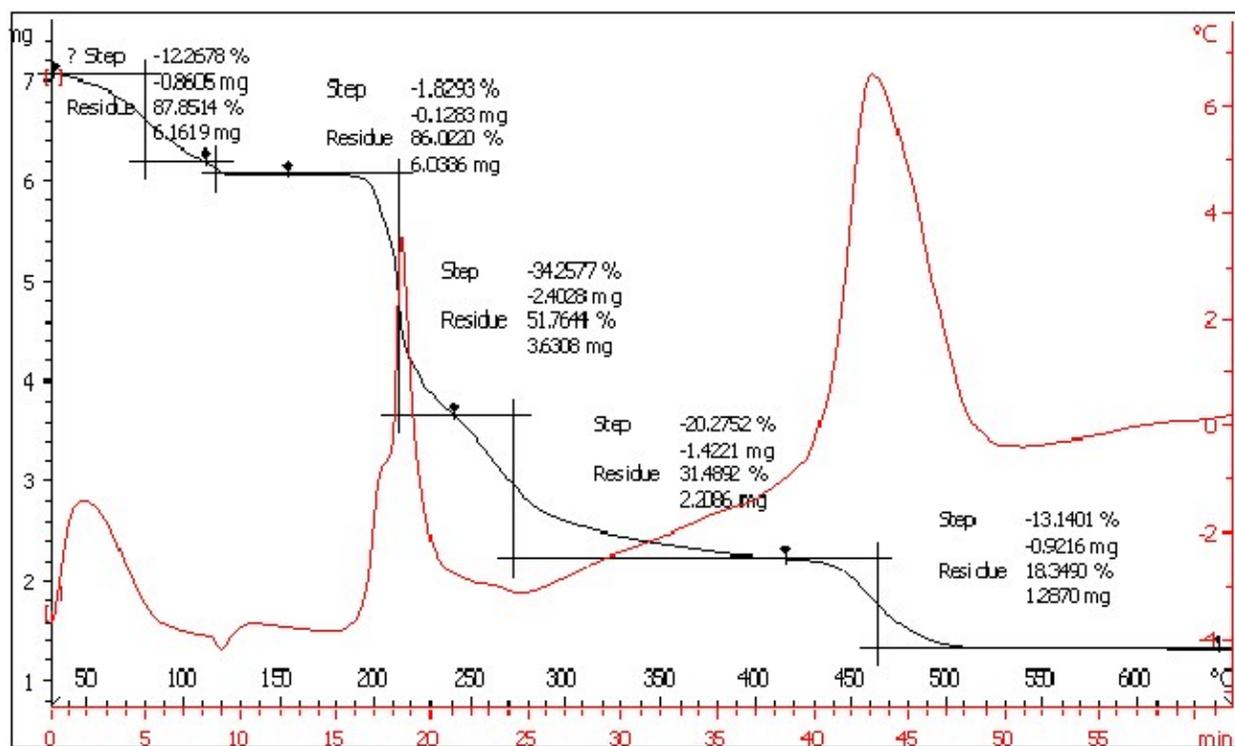


Figure S7: The TG-DTA curve of complex 2

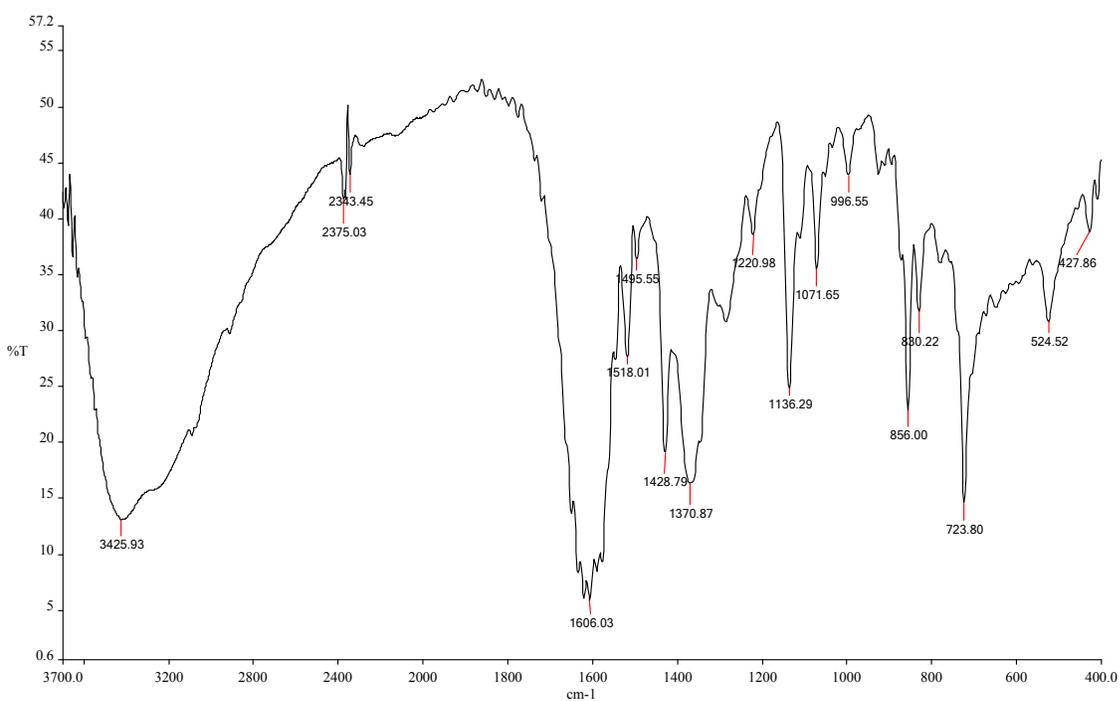
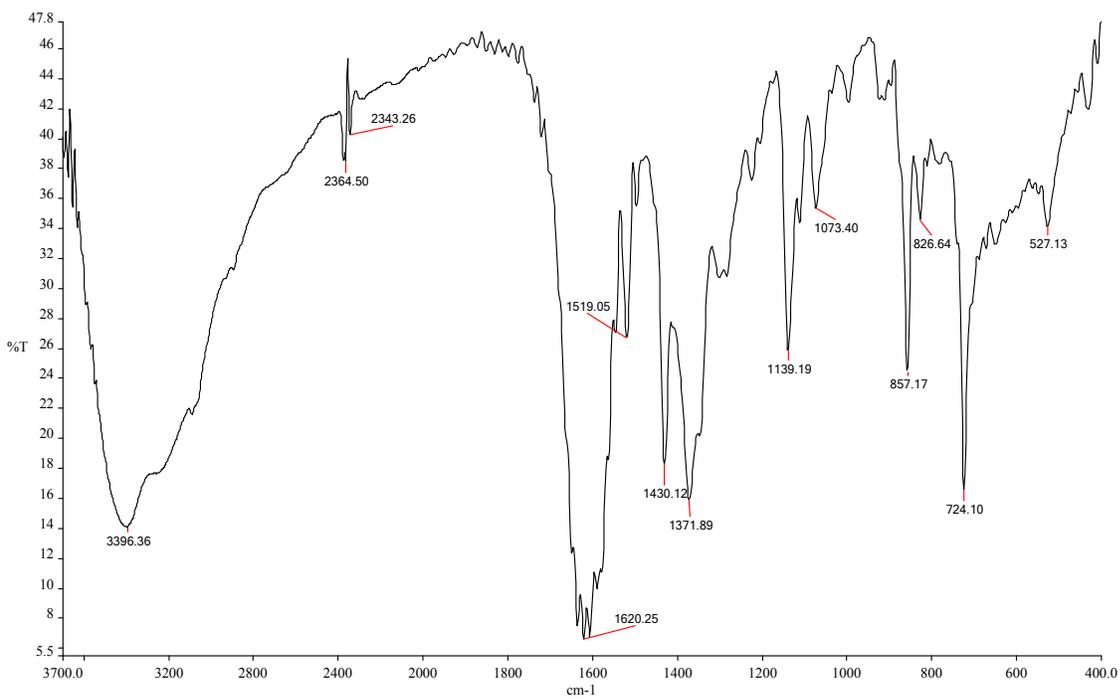
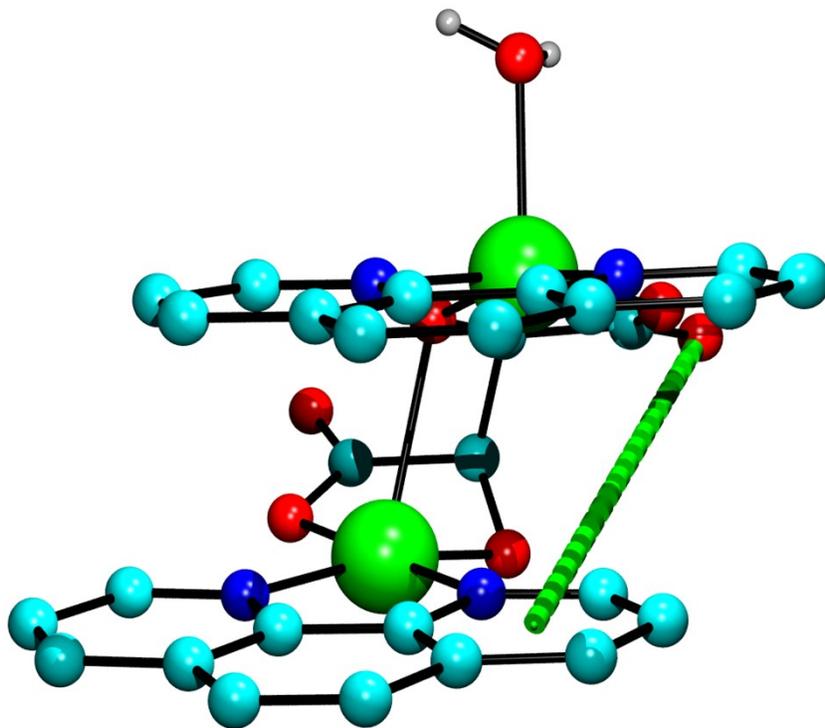


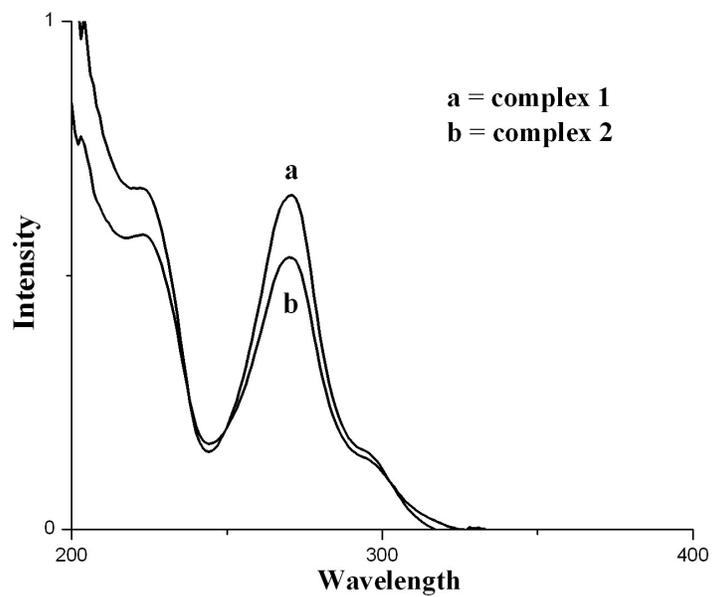
Figure S8: IR data of Complex 1



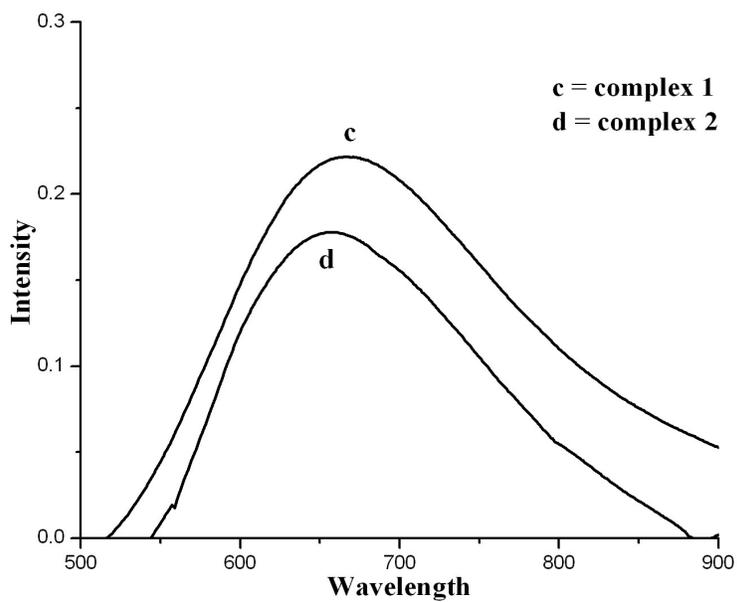
**Figure S9:** IR data of complex 2



**Figure S10:** Oxygen- $\pi$  interaction between O6 oxygen atom and  $\pi$ -ring (cg7) in complex1



(a)



(b)

**Figure S11:** The UV-Vis spectra of the two complexes at two different wavelength region [(a) low concentration at low wavelength region, (b) high concentration at longer wavelength region].

