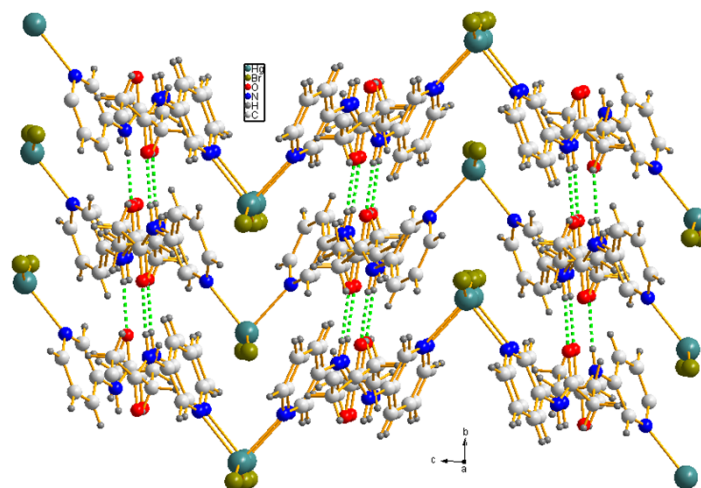


**Electronic supplementary information (ESI)**

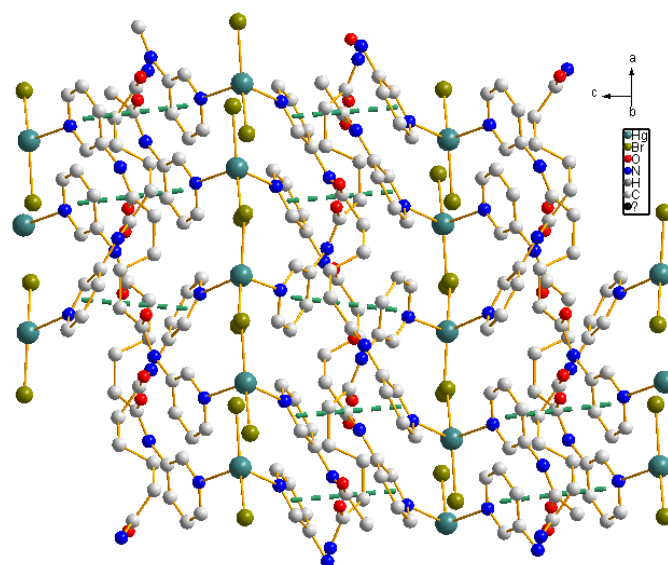
**Hg(II) supramolecular isomers:  
structural transformation and photoluminescence change**

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Taiwan, R.O.C.*

**Fig. S1** (a) A drawing showing the N–H---O interactions in **1**. (b) A drawing showing the shortest  $\pi$ - $\pi$  contact.

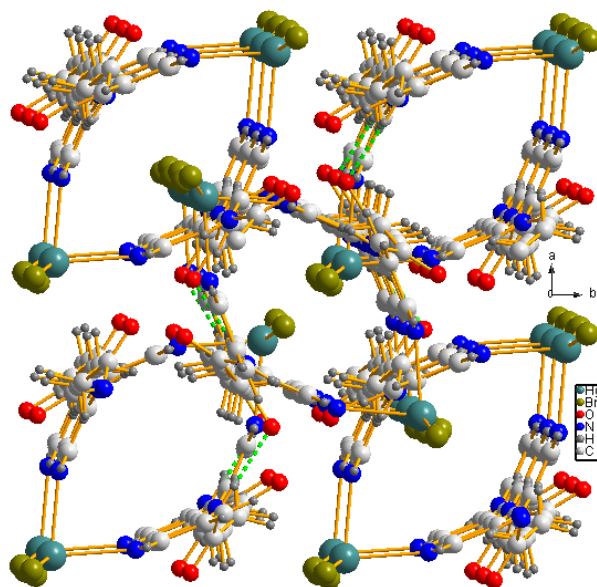


**(a)**

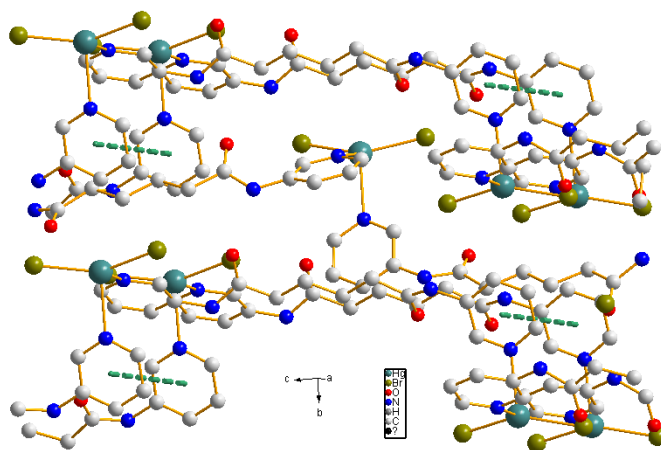


**(b)**

**Fig. S2** (a) A drawing showing the N–H---O interactions in **2**. (b) A drawing showing the shortest  $\pi$ - $\pi$  contact.

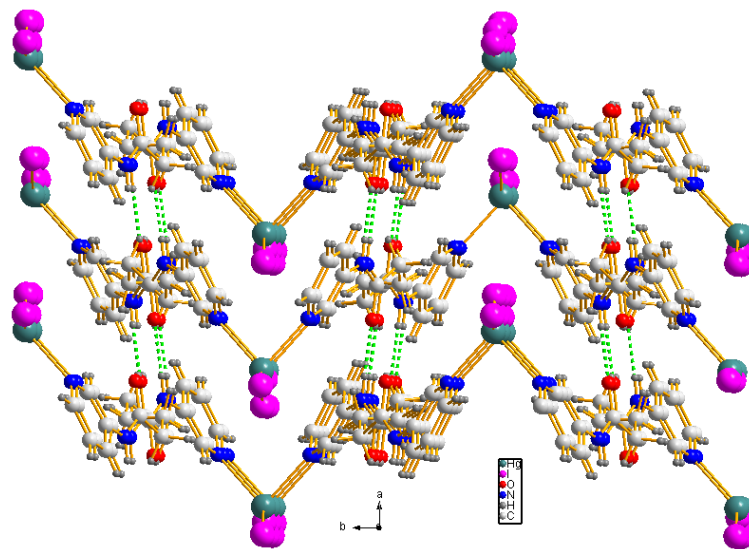


**(a)**

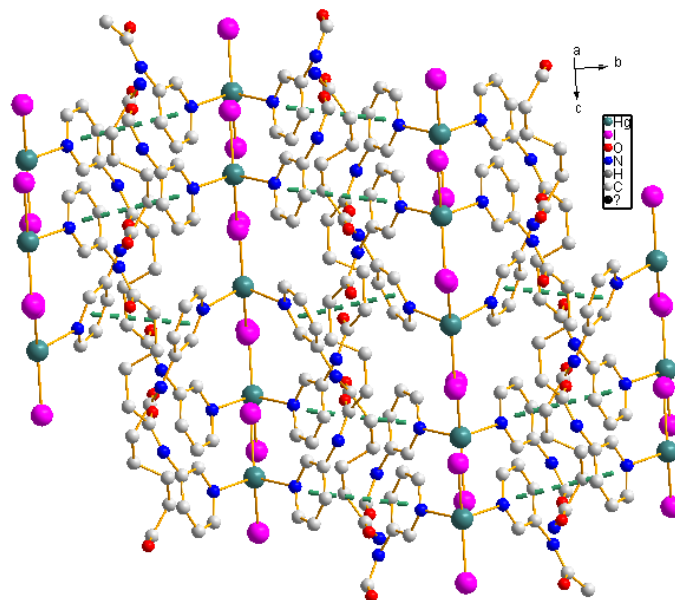


**(b)**

**Fig. S3** (a) A drawing showing the N–H---O interactions in **3**. (b) A drawing showing the shortest  $\pi$ - $\pi$  contact.

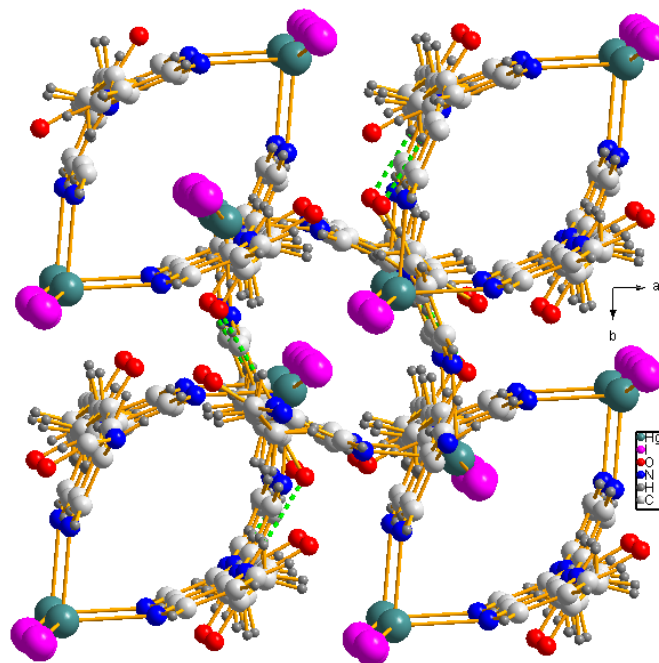


**(a)**

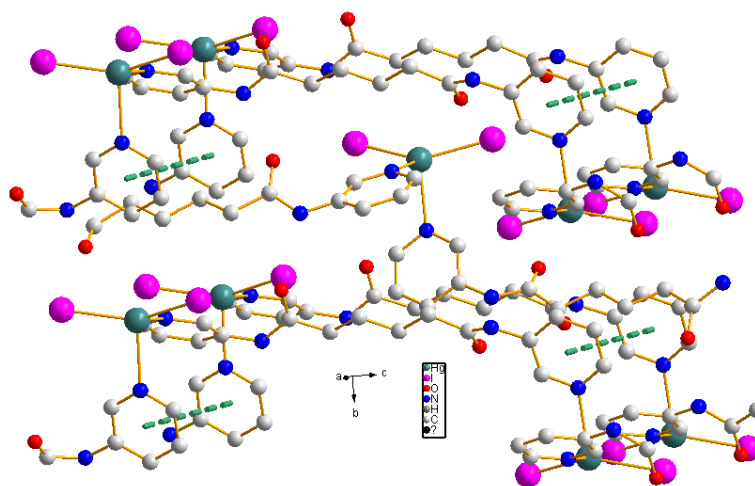


**(b)**

**Fig. S4** (a) A drawing showing the N–H---O interactions in **4**. (b) A drawing showing the shortest  $\pi$ - $\pi$  contact.

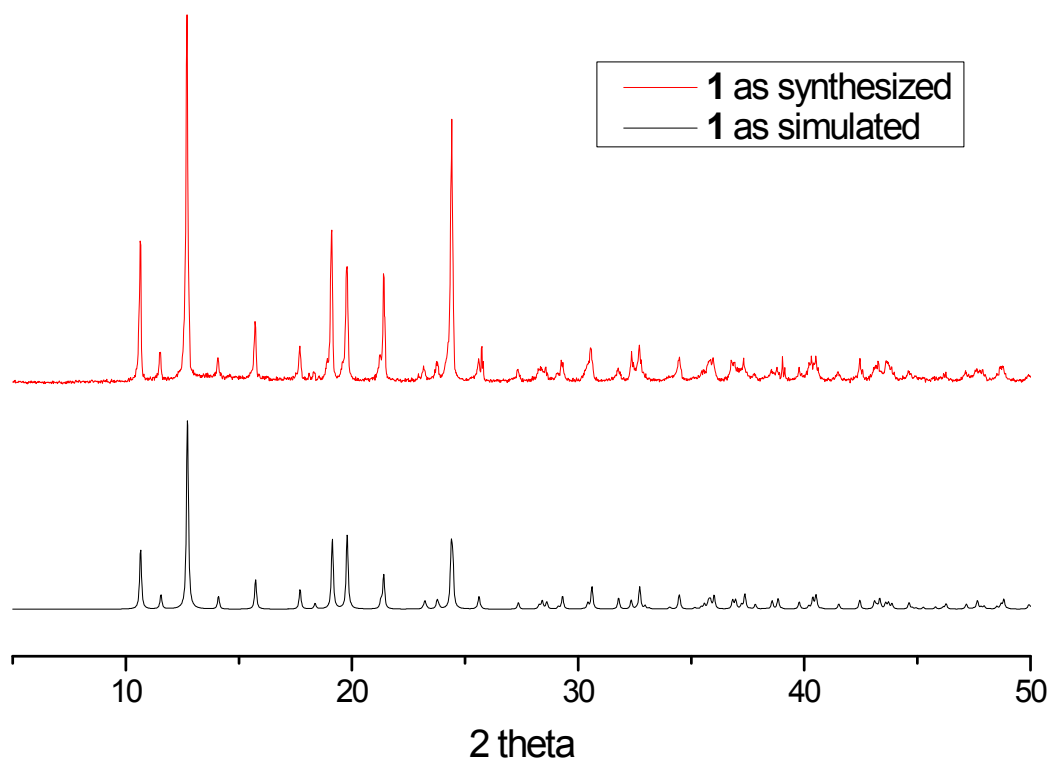


**(a)**

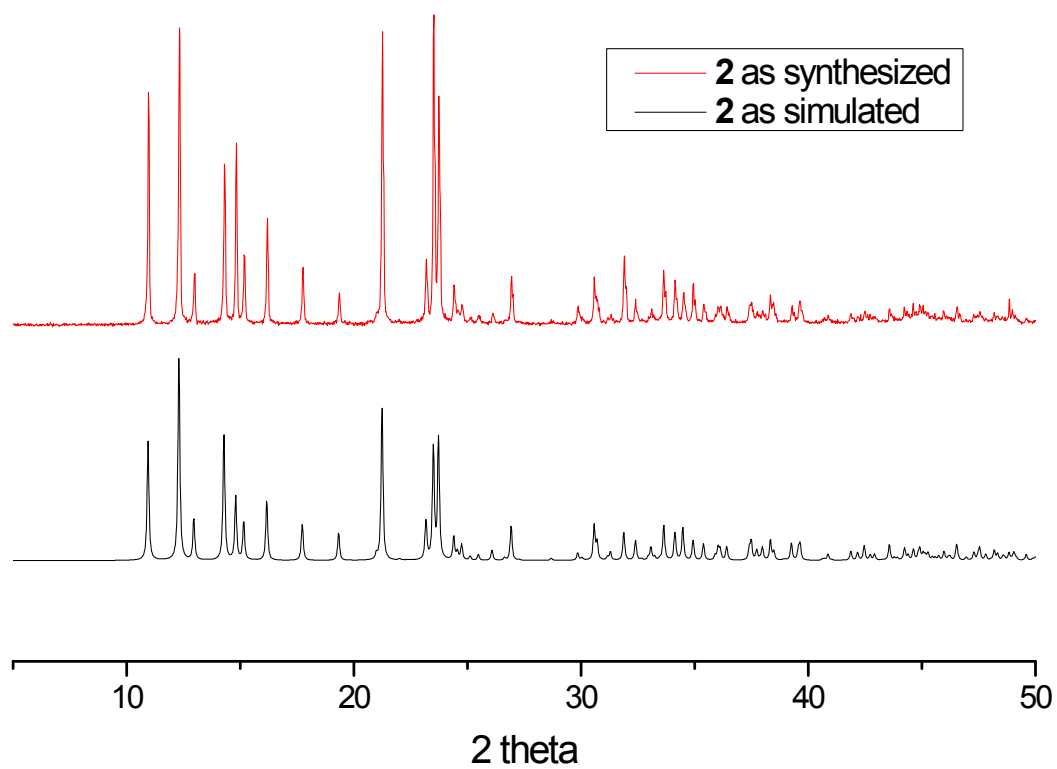


**(b)**

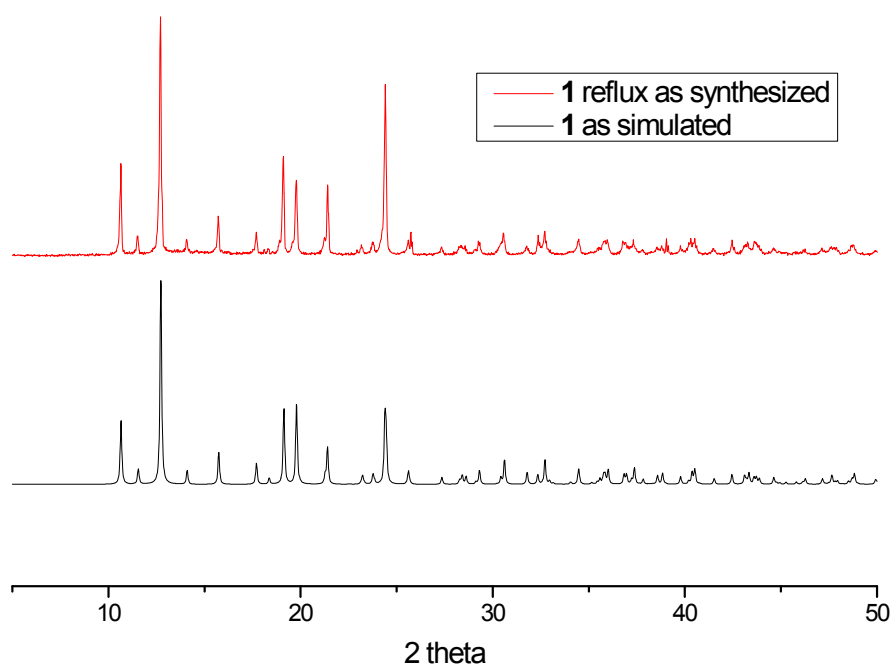
**Fig. S5** Simulated and experimental powder X-ray patterns for **1**.



**Fig. S6** Simulated and experimental powder X-ray patterns for **2**.

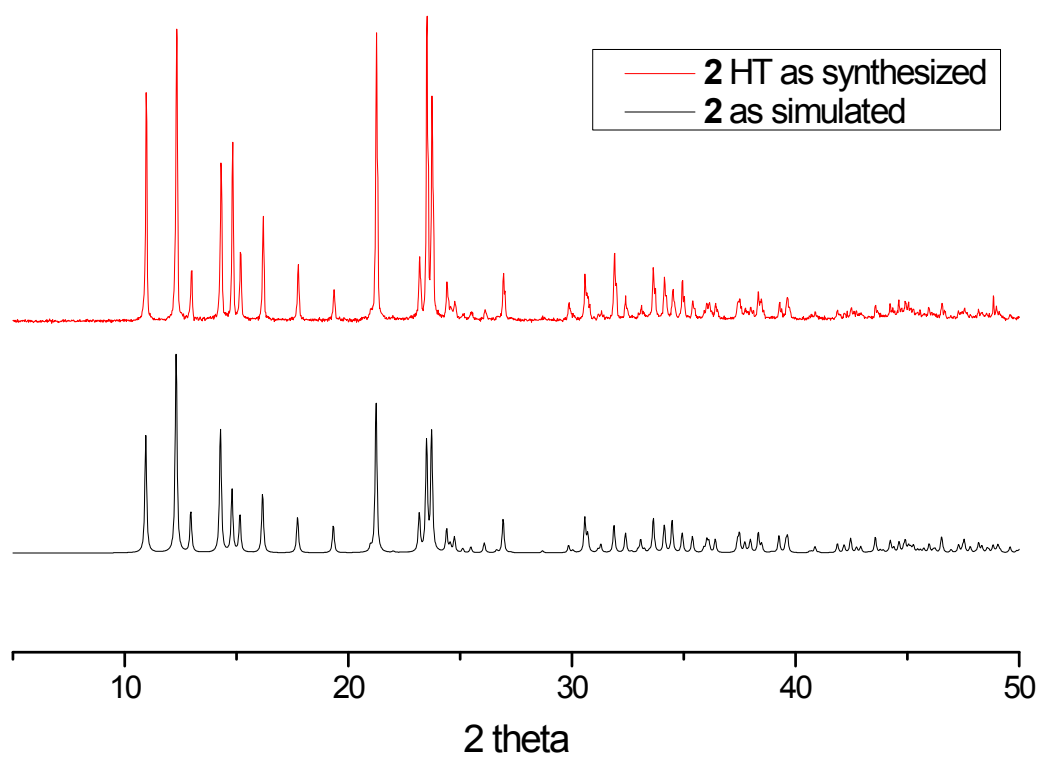


**Fig. S7** Simulated and experimental powder X-ray patterns for **1** (alternate method).

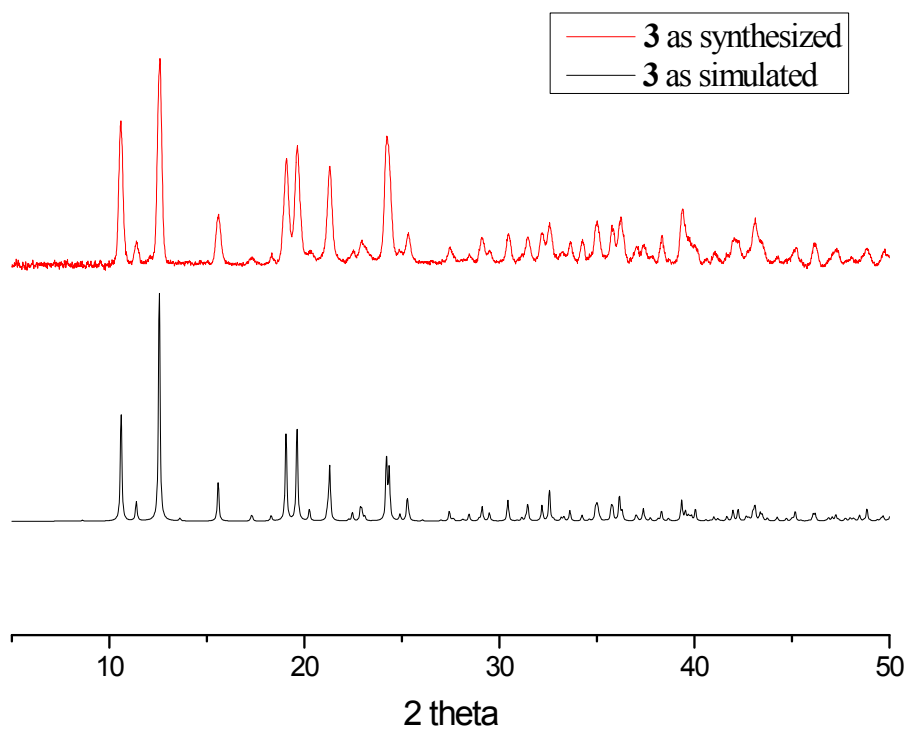




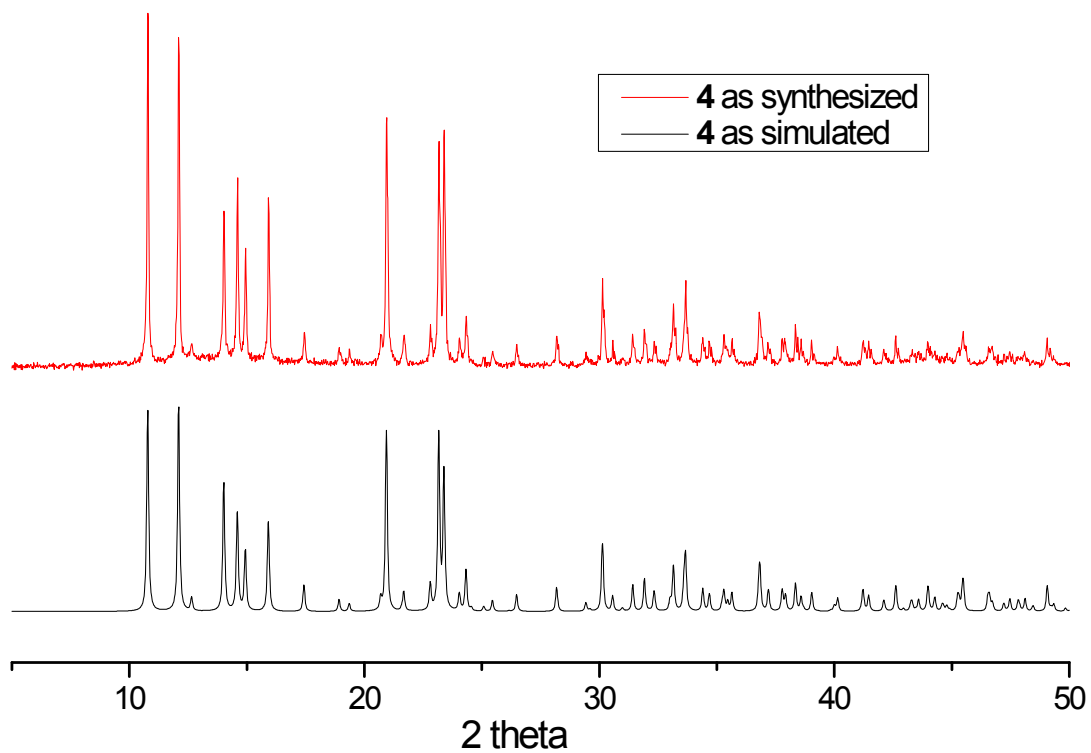
**Fig. S8** Simulated and experimental powder X-ray patterns for **2** (alternate method).



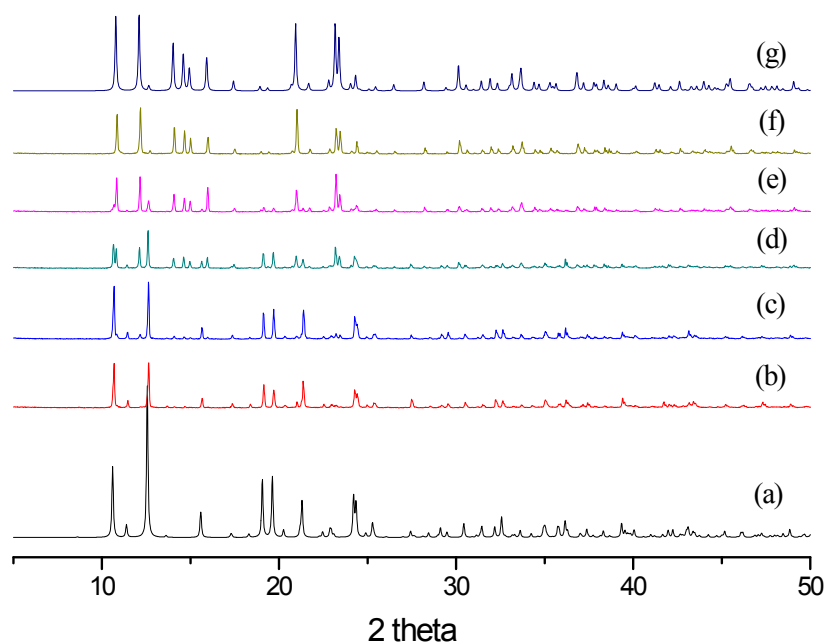
**Fig. S9** Simulated and experimental powder X-ray patterns for **3**.



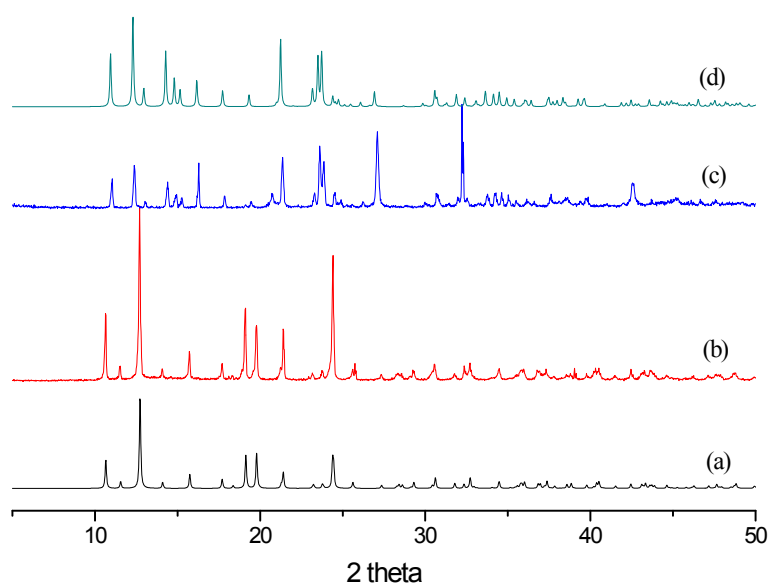
**Fig. S10** Simulated and experimental powder X-ray patterns for **4**.



**Fig. S11** (a) Powder XRD pattern of **3** at variable temperature showing crystal to crystal transformation: (a) simulation of **3**, (b) RT, (c) 180 °C, (d) 190 °C, (e) 200 °C (f) 210 °C and (g) simulation of **4**. (b) Powder XRD patterns showing structural transformation from complex **1** to **2** under hydrothermal condition: (a) simulation of **1**, (b) **1** as synthesized, (c) **2** after hydrothermal and (d) simulation of **2**.

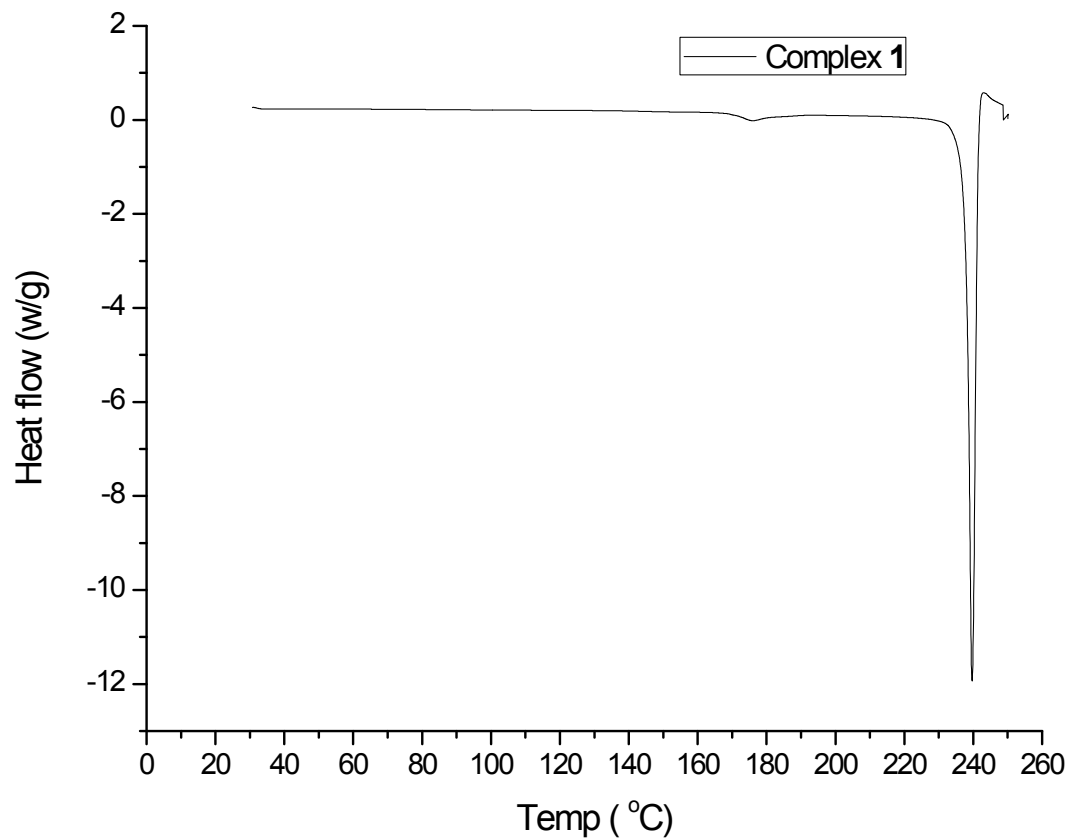


**(a)**

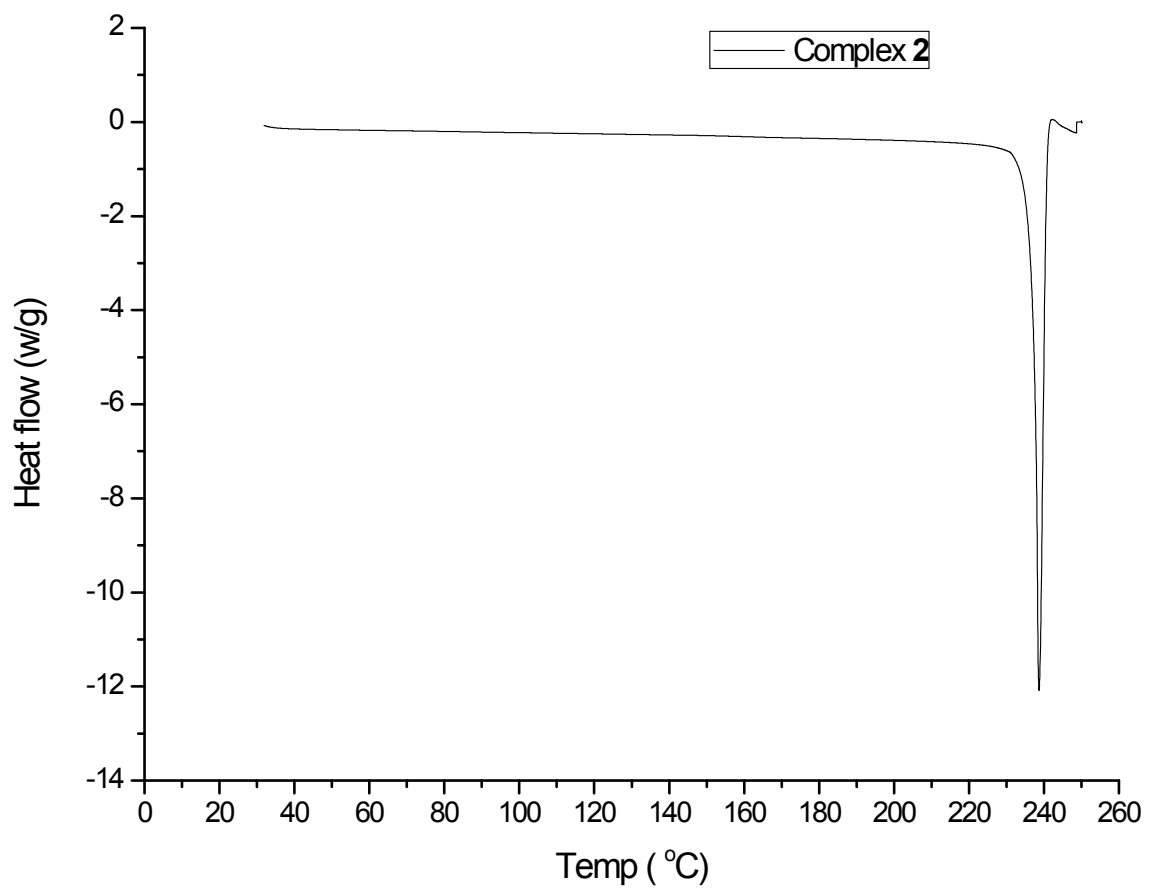


**(b)**

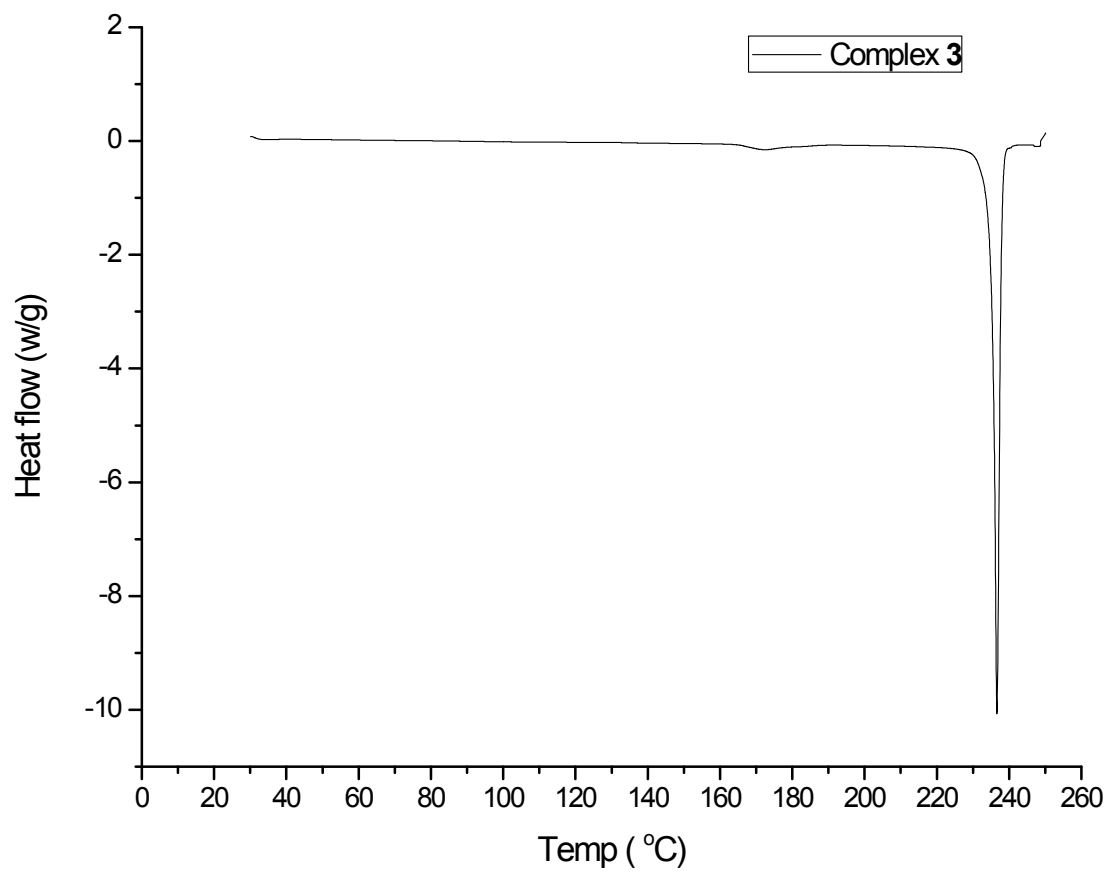
**Fig. S12** DSC thermogram of complex **1**.



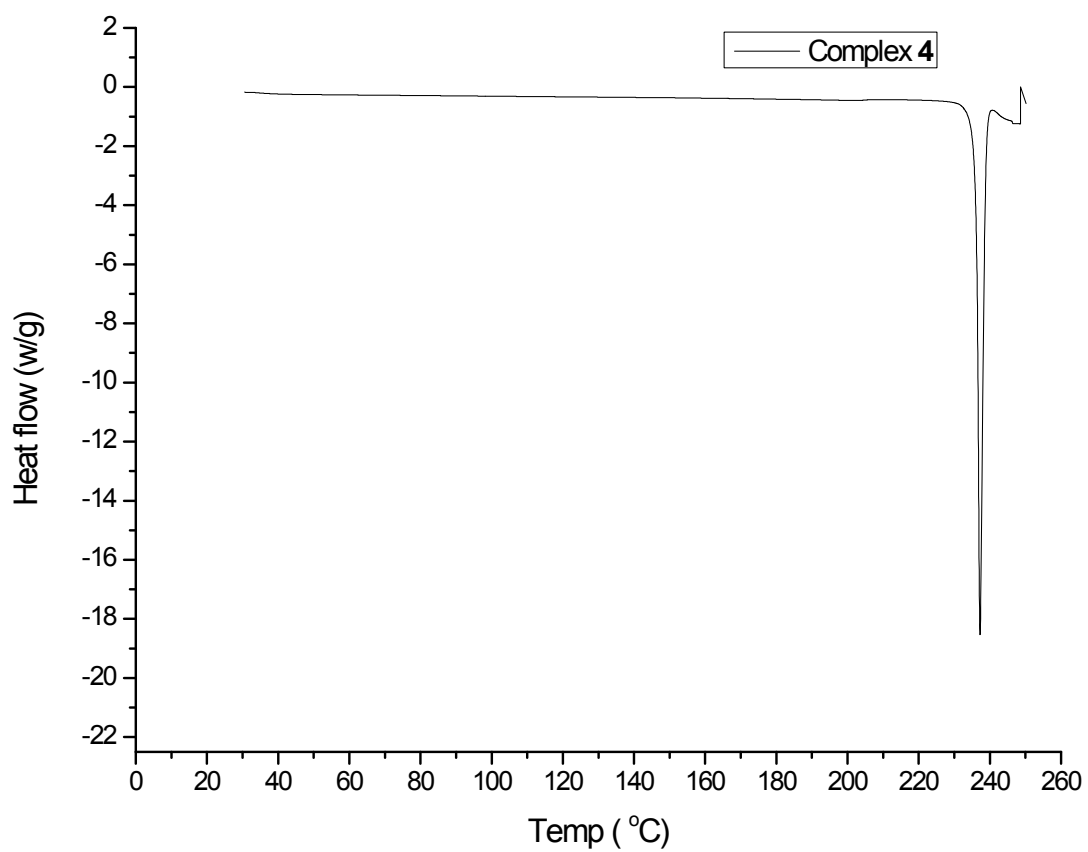
**Fig. S13** DSC thermogram of complex **2**.



**Fig. S14** DSC thermogram of complex **3**.

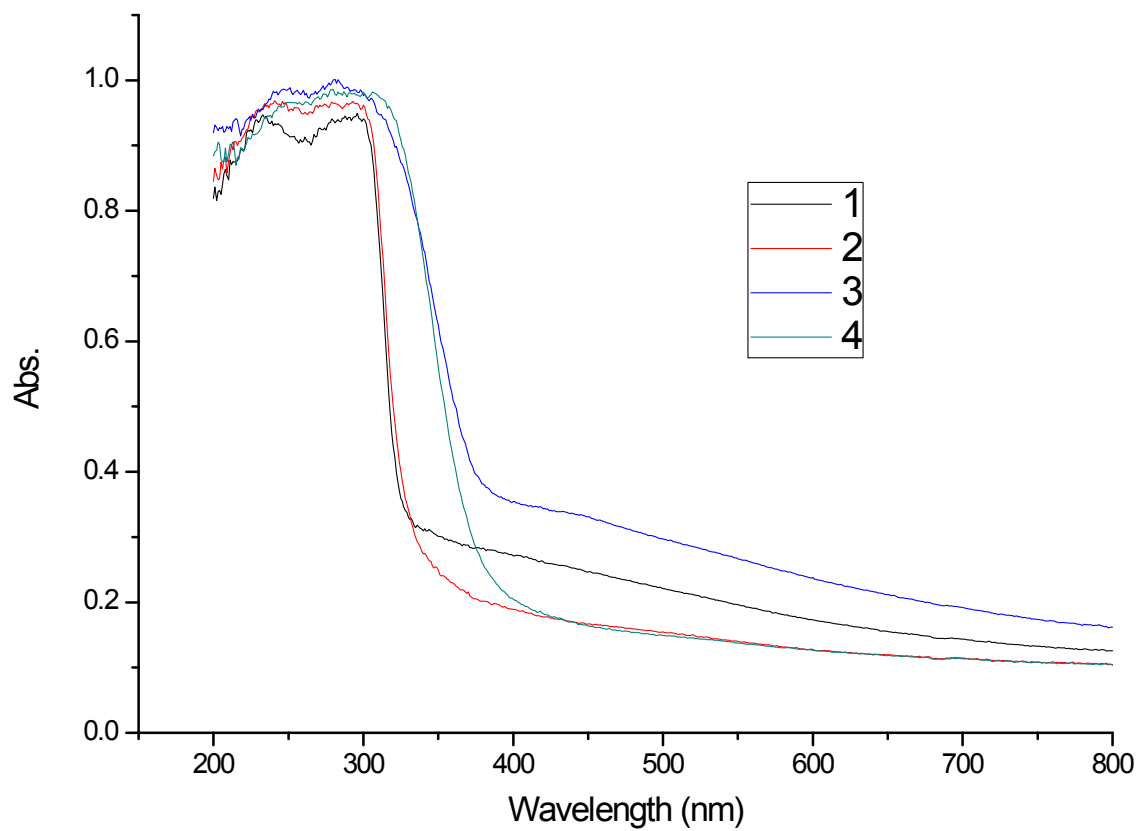


**Fig. S15** DSC thermogram of complex 4.

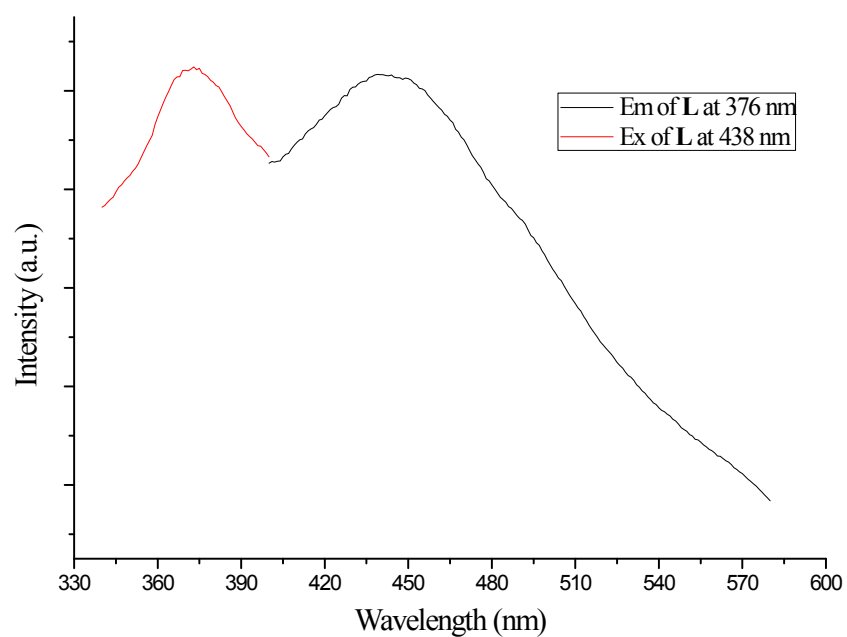




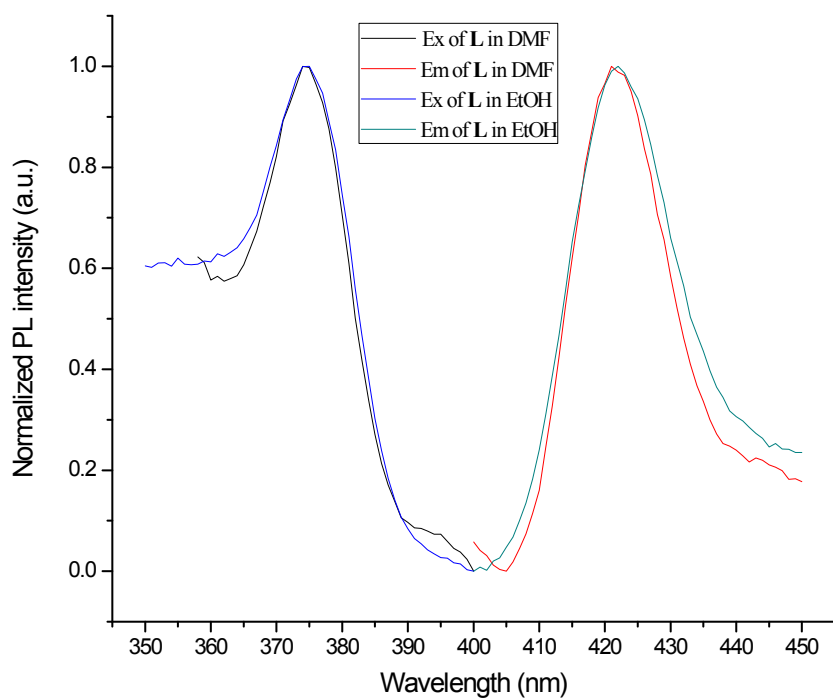
**Fig. S16** Solid state UV/Visible spectra of **1- 4**.



**Fig. S17** (a) Solid and (b) solution (0.5 mM in DMF and EtOH) emission/excitation spectra of **L** ligand.



**(a)**



**(b)**

Ligand	Solvent	Ex (nm)	Em (nm)
<b>L</b>	DMF	374	421
<b>L</b>	EtOH	375	422

**Fig. S18** Normalized emission spectra of **1-3** in the solid state.

