

## **Electronic Supporting Information**



Fig. S1 <sup>1</sup>H NMR spectrum of hnbdtiH (500 MHz, CDCl<sub>3</sub>).



Fig. S2 <sup>1</sup>H NMR spectrum of 1 (500 MHz, CDCl<sub>3</sub>).



Fig. S3 <sup>1</sup>H NMR spectrum of 2 (500 MHz, CDCl<sub>3</sub>).



Fig. S4 Experimental and simulated XRD patterns of hnbdtiH.



Fig. S5 Experimental and simulated XRD patterns of 1.



Fig. S6 Experimental and simulated XRD patterns of 2.



**Fig. S7** Molecular structure of hnbdtiH (50% probability). All H atoms attached to C atoms are omitted for clarity.



Fig. S8 Packing structure of 2.



**Fig. S9** The morphology of **1** in CH<sub>3</sub>CN–H<sub>2</sub>O mixture (v/v = 1/1, c =  $2 \times 10^{-5}$  M), showing particles with a size range of 200-300 nm.



Fig. S10 Particle size distributions of 1 in CH<sub>3</sub>CN–H<sub>2</sub>O mixture (v/v = 1/1, c = 2 ×  $10^{-5}$  M).



Fig. S11 Luminescence spectra of 2 in  $CH_3CN-H_2O$  mixtures with different water fractions.