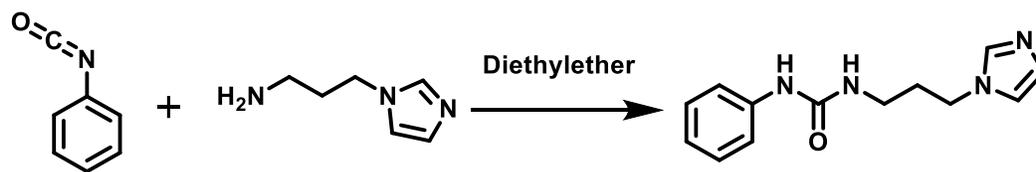


Supporting Information

Consequences of Twisting of flexible arms of imidazole derived urea in zinc-dicarboxylate coordination polymers

Satyendra Verma, Rinki Brahma and Jubaraj B. Baruah*



Scheme 1S: Reaction for the synthesis of the *imidaurea*

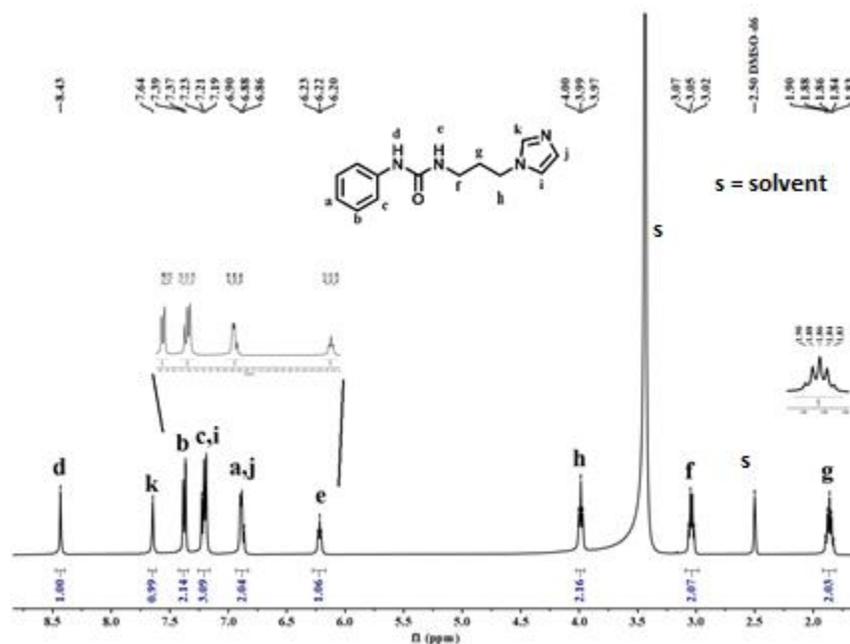


Figure 1S: ¹H NMR spectra (500 MHz, DMSO-d₆) of the *imidaurea*.

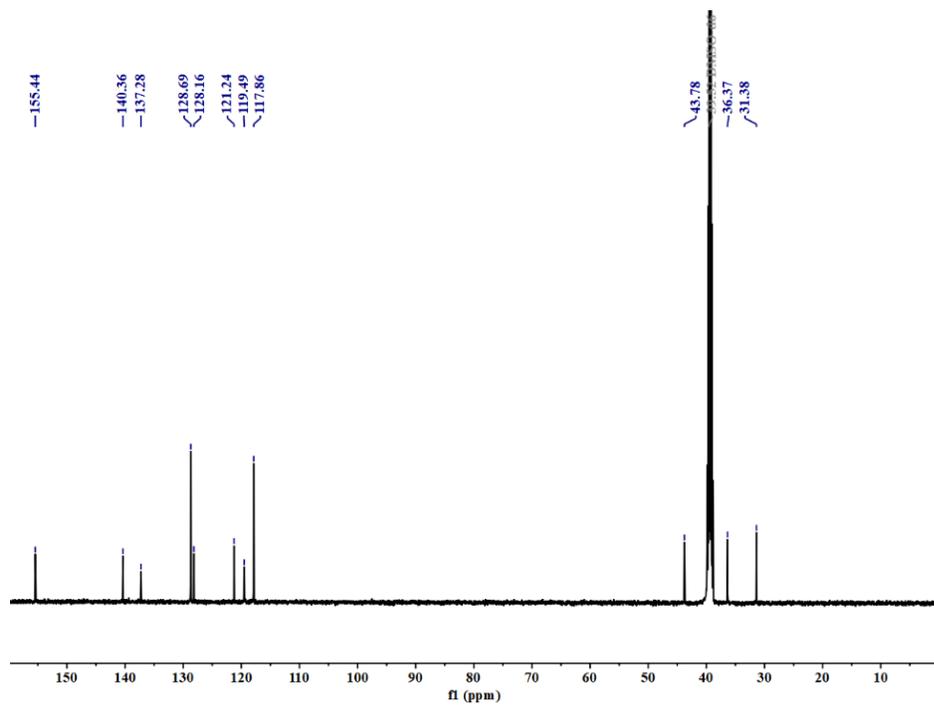


Figure 2S: ^{13}C NMR (DMSO- d_6 , 125 MHz) spectra of the *imidaurea*.

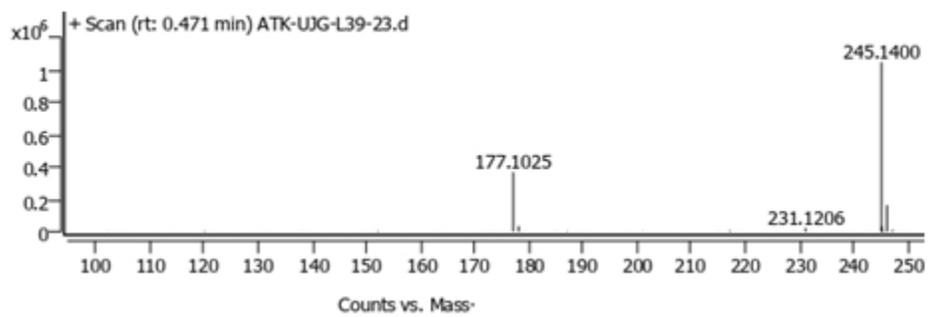


Figure 3S: High resolution mass spectra of *imidaurea*

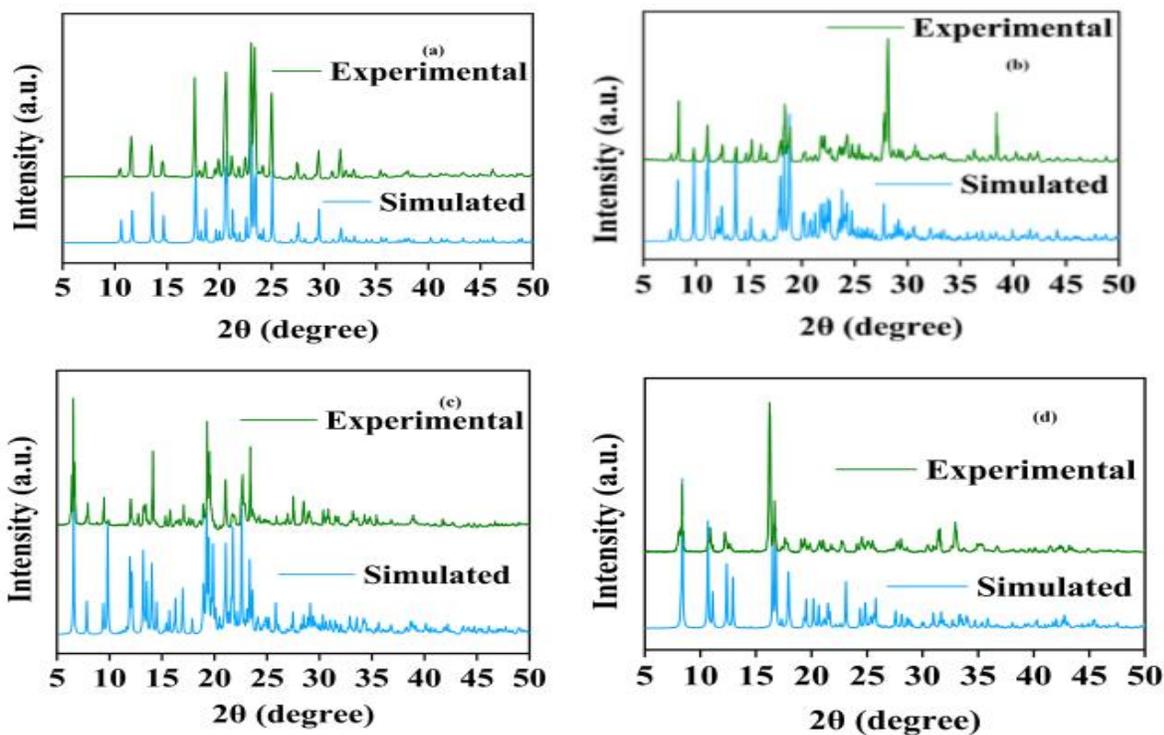


Figure 4S: Powder X-ray diffraction patterns of the (a) *imidaurea*, (b) CP1, (c) CP2, (d) CP3 (Green = Experimental, Blue = Simulated). Simulated pattern generated from CIF file).

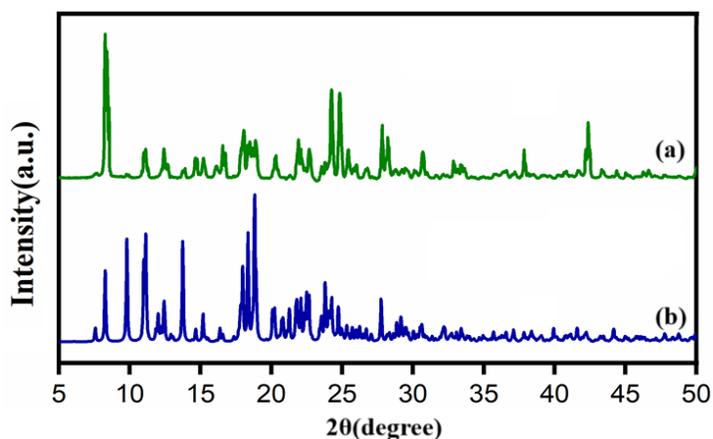


Figure 5S : Powder X-ray diffraction patterns of (a) CP2 after heating at 150° C for two days, and (b) simulated pattern of CP1.

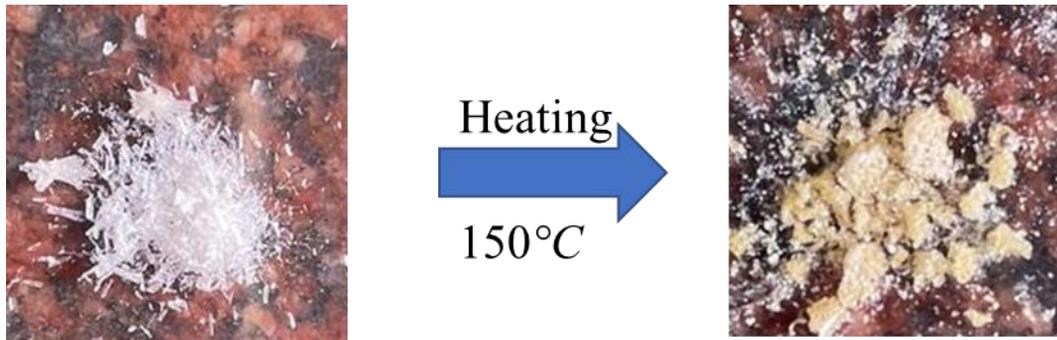


Figure 6S: Photographs of the CP2 and of the CP2 heat treated at 150° C for two days.

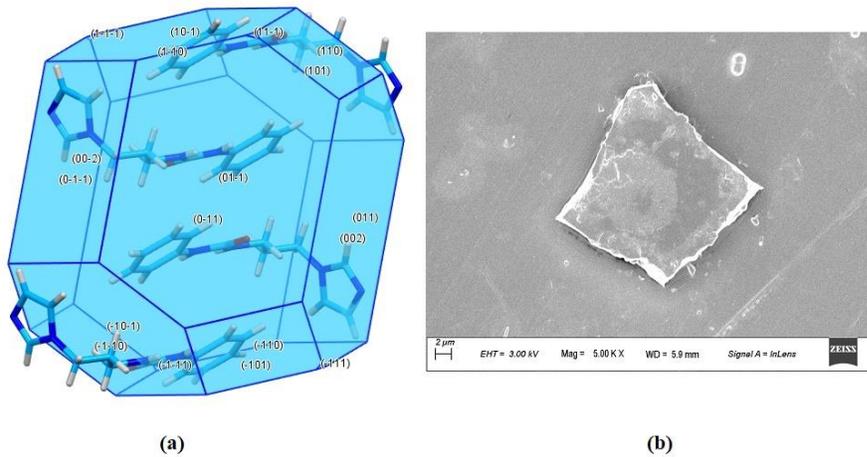
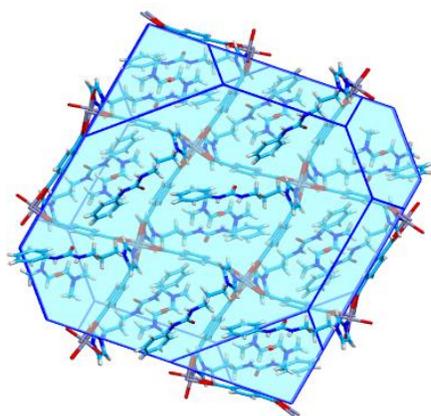
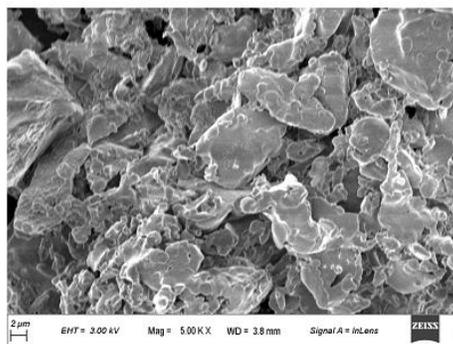


Figure 7S : (a) Bravais, Friedel, Donnay and Harker crystal morphology of *imidaurea*; (b) scanning electron microscopy image of the *imidaurea*.



(g)



(h)

Figure 10S : (a) Bravais, Friedel, Donnay and Harker crystal morphology of **CP3**; (b) scanning electron microscopy image of the **CP3**.

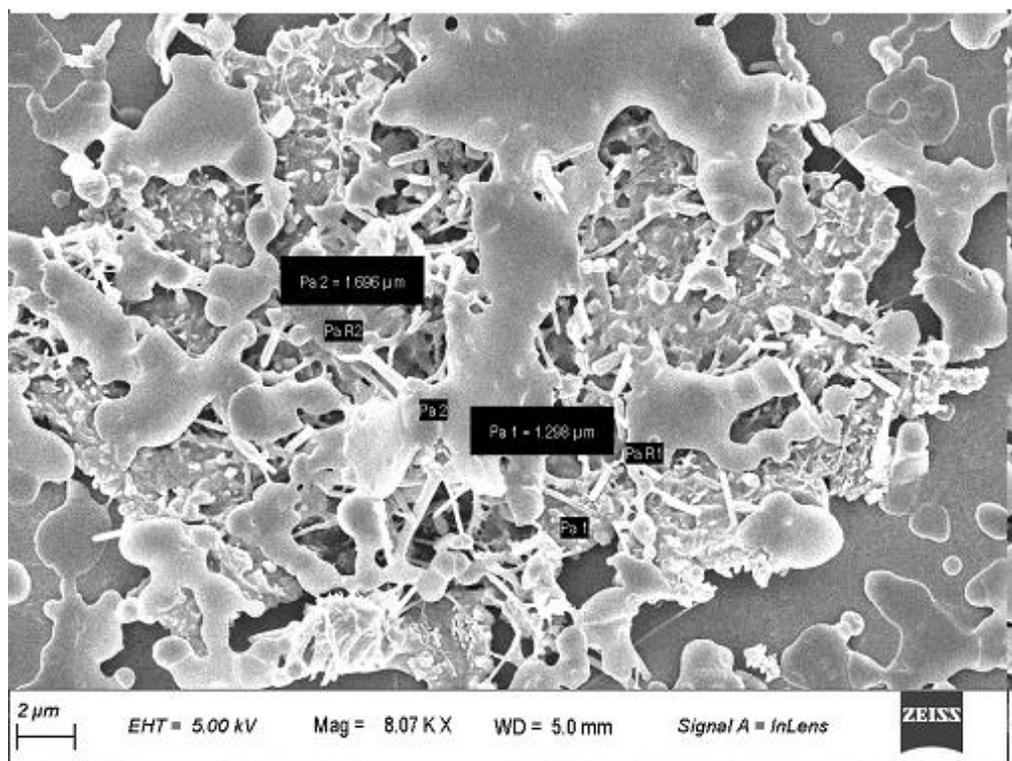
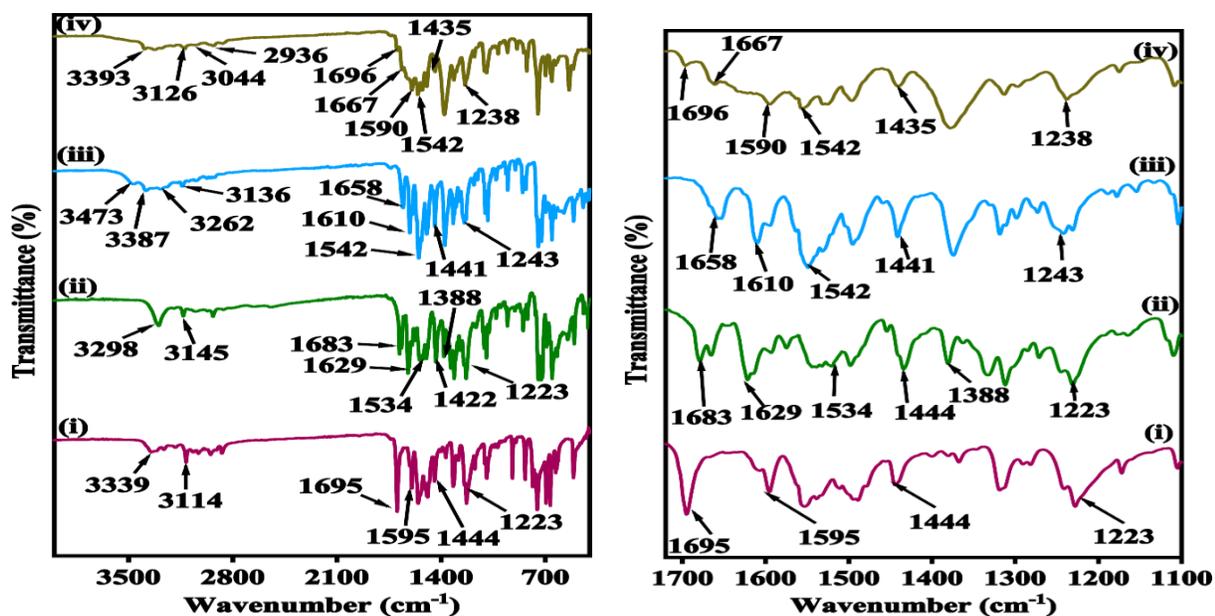
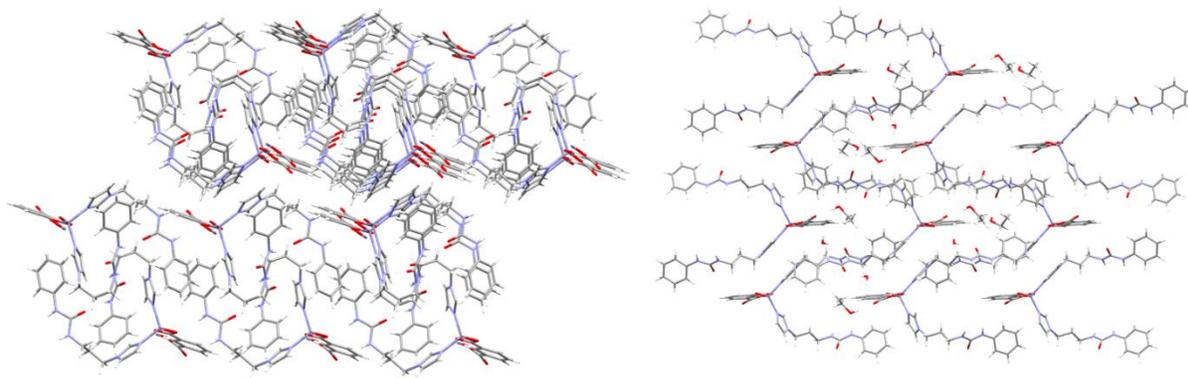


Figure 11S: Scanning electron microscopic image of heat treated at 150° C for two days of **CP2**.



(b)

Figure 12S: (a) IR-spectra, and (b) expansion of the IR-spectra of the solid samples of (i) *imidaurea*, (ii) CP1, (iii) CP2, (iv) CP3.



(b)

Figure 13S: Packing patterns showing (a) layer-like assemblies of bunches in the CP1, and (b) inter-chain inclusion in clefts in chains in the CP2.

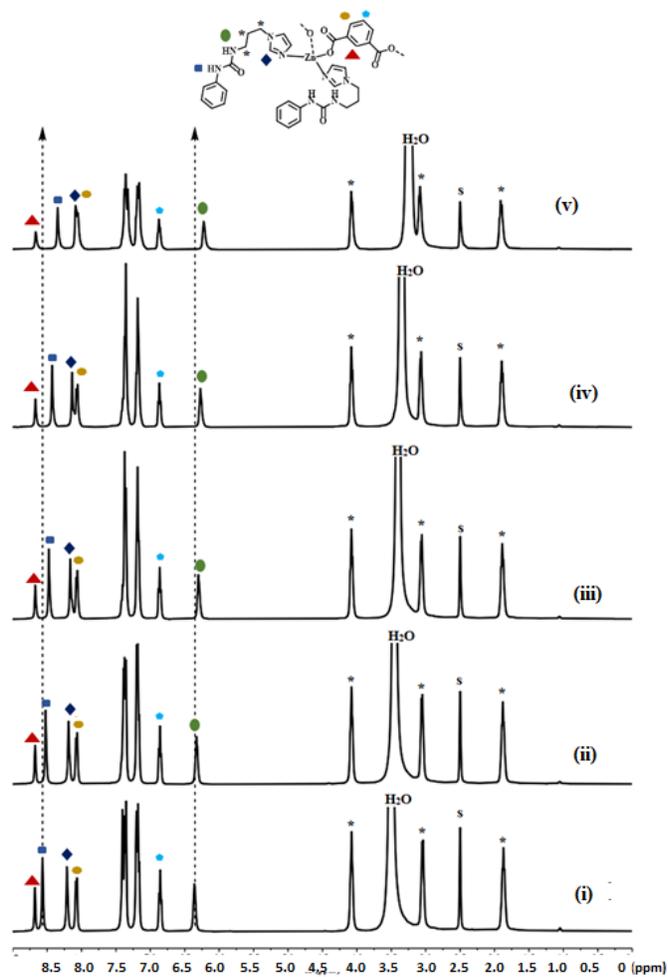


Figure 14S: ^1H NMR spectra (500 MHz) of the **CP1** in DMSO-d_6 at (a) 293.15K, (b) 303.15K, (iii) 313.15K, (iv) 323.15K, (v) 333.15K.

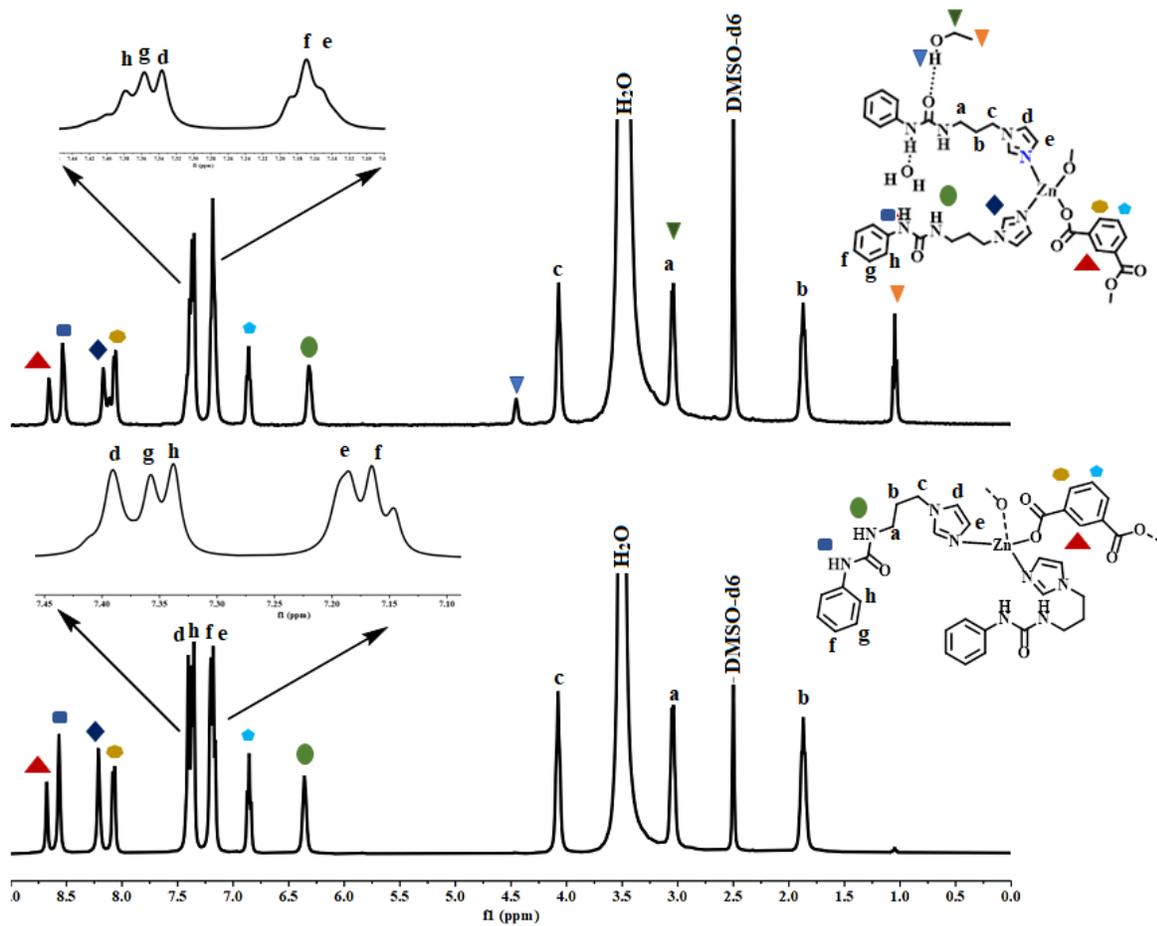


Figure 15S: $^1\text{H NMR}$ (500MHz) of the CP1 and CP2 in DMSO-d_6

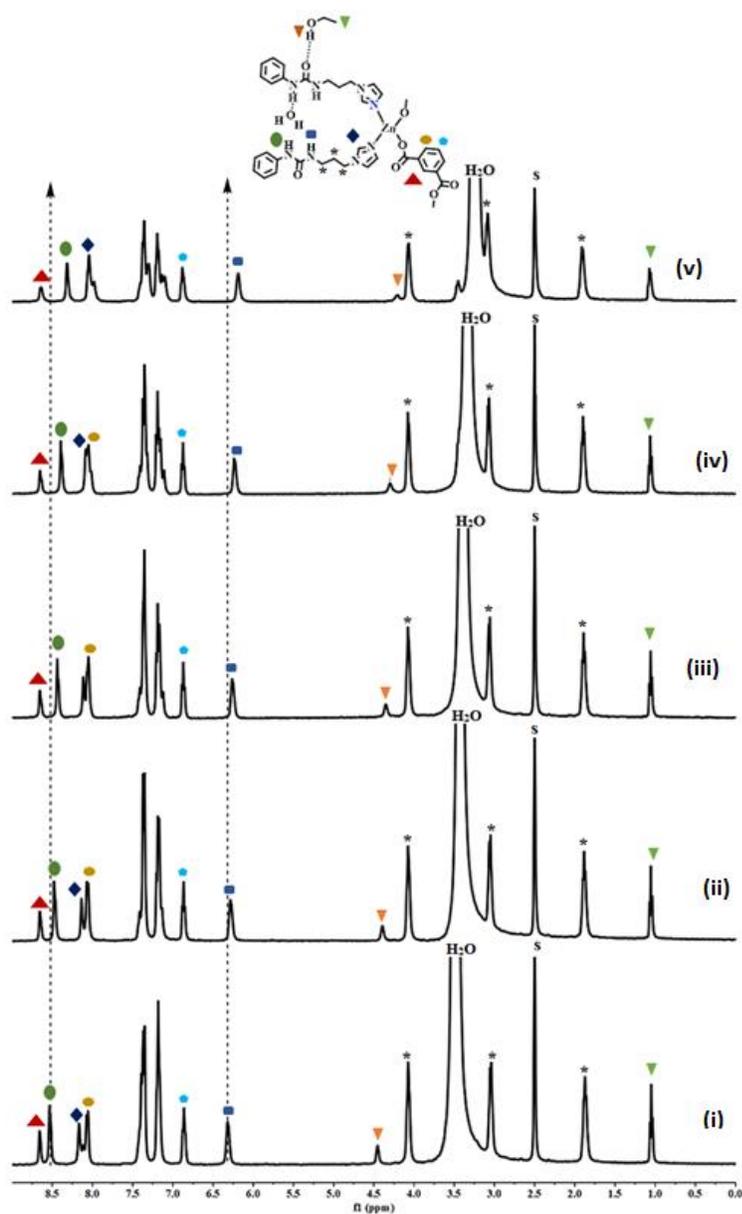


Figure 16S: ^1H NMR spectra (500 MHz) of the **CP2** in DMSO-d_6 at (a) 293.15K, (b) 303.15K, (iii) 313.15K, (iv) 323.15K, (v) 333.15K.

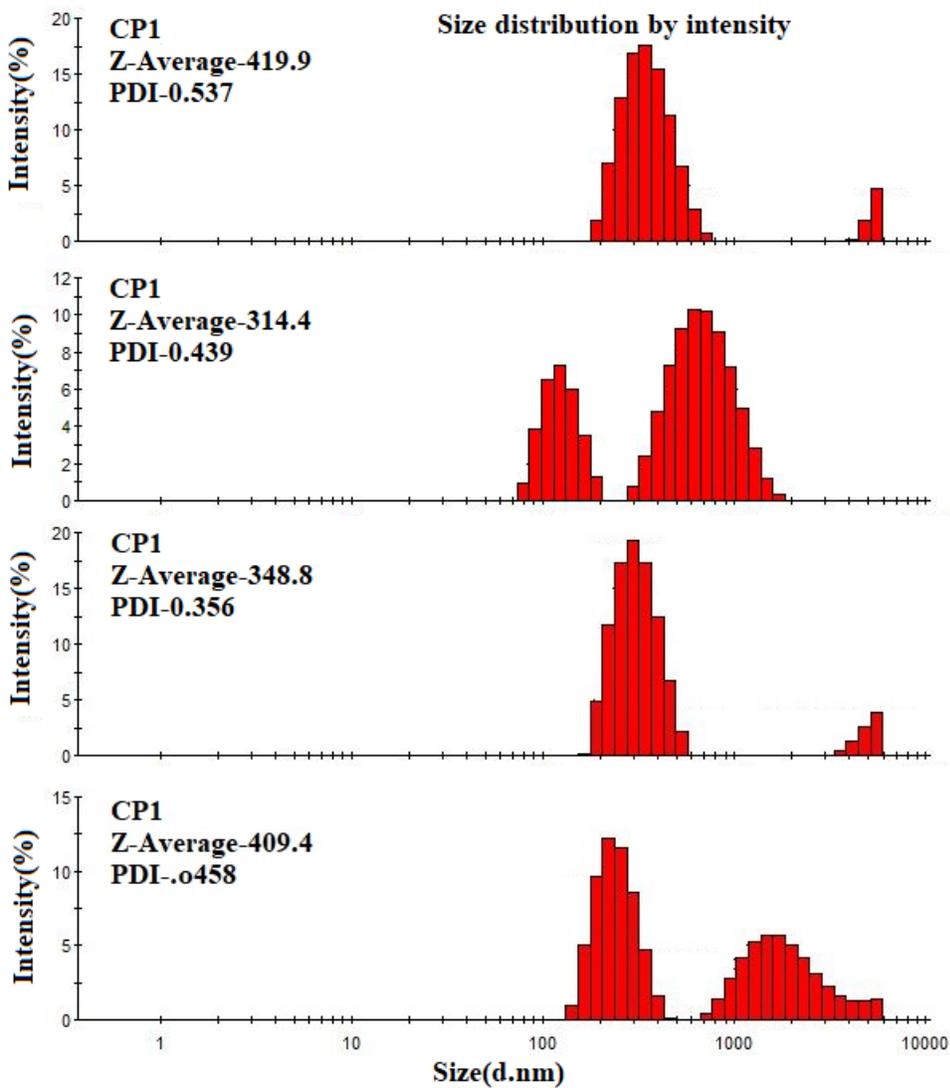


Figure 17S: Plots of intensity vs particle size from dynamic light-scattering of the CP1 (80 μL of 10⁻⁴M) with different concentrations of isophthalic acid (0μL, 10μL,20μL,30μL 10⁻⁴M, bottom to top) in water.

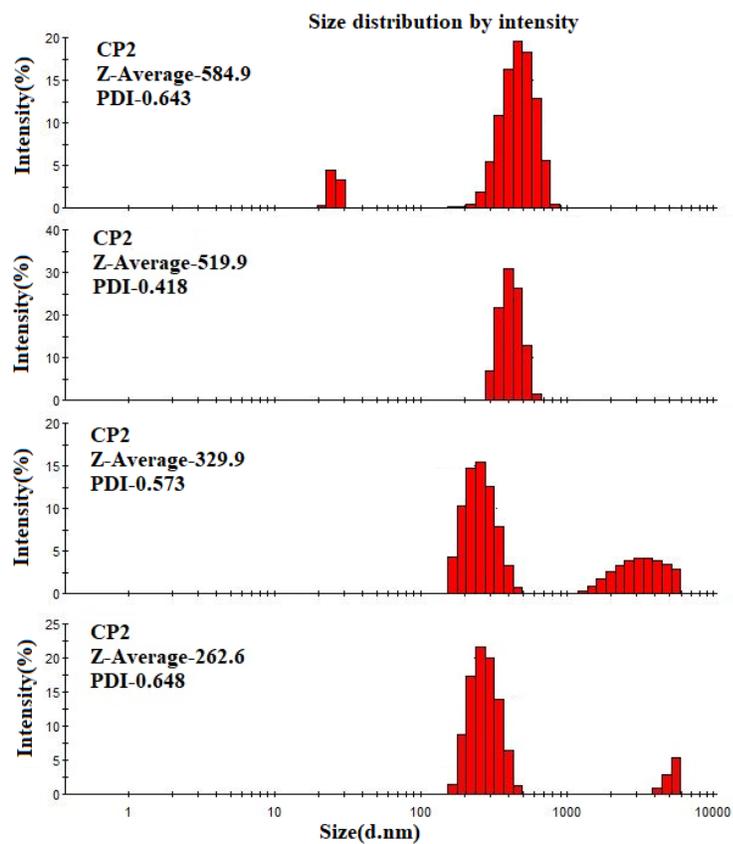


Figure 18S: Plots of intensity vs particle size determined from dynamic light-scattering of **CP2** (80 μL of 10^{-4}M) with different concentrations of isophthalic acid (0 μL , 10 μL , 20 μL , 30 μL 10^{-4}M , bottom to top) in water.