## Supporting information

## Reversible phase transformations upon water uptake/removal in crystalline material of a bipodal N-donor ligand and evaluation of the stability of the hydrates formed

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**Fig. S1** Overlays of the ligands: 1/2, 1/3 and 1/4, 1 (red), 2 (light green), 3 (blue), and 4 (yellow); the RMS deviations (after inversion) are as follows: 0.6794, 0.3927, 0.7943 Å.



**Fig. S2** Experimental PXRD patterns obtained for the products isolated from different solvents and simulated traces generated for **1-4**.



Fig. S3 Thermogram of the bulk hydrated ligand sample.



**Fig. S4** On the left: photo of anhydrous bulk material upon immersion in water; on the right: photo of the same material after leaving it for 17h in water, indicating recrystallization.