Supporting Information

Extending the Supramolecular Synthon Concept in Flexible Polyaminocarboxylate based Coordination Polymers

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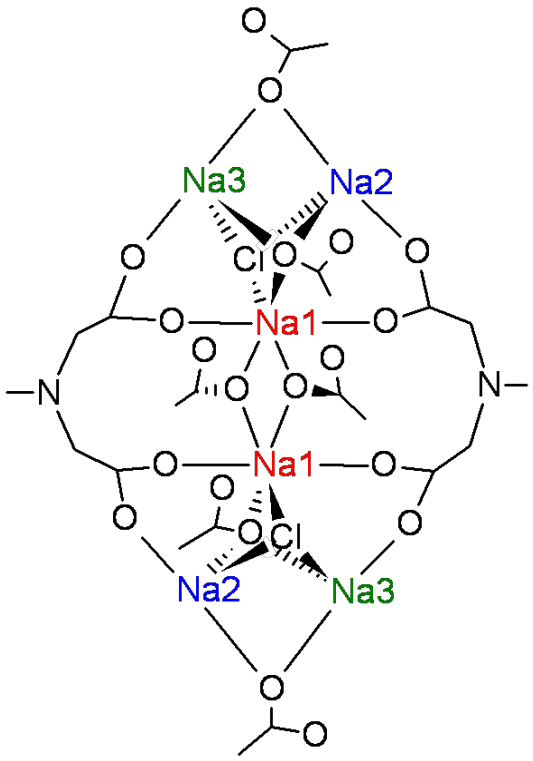


Scheme S1. Sodium ions cluster linking eight TTHA ions in solid **1**.

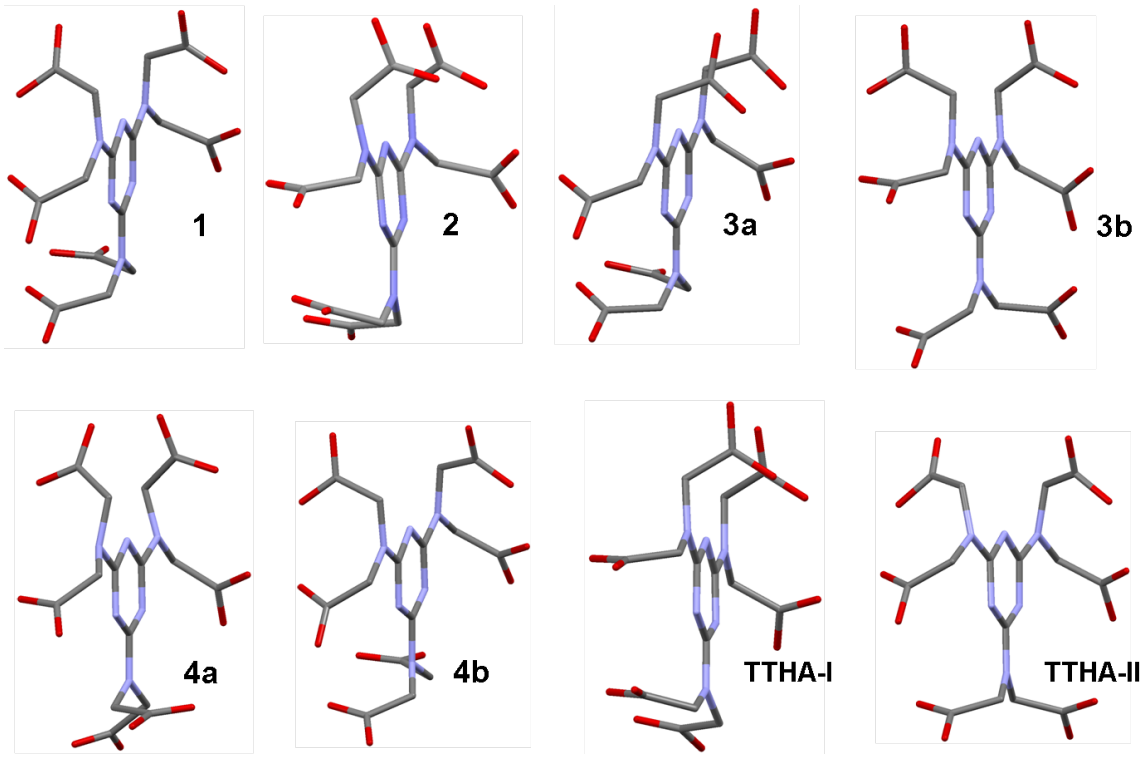


Figure S1. TTHA conformations in the crystal structures of solids **1** through, **4** and TTHA polymorph I and II. Notice that only four distinct conformations can be seen in the eight structures mentioned: type I is found in **1** and **4b**; type II in **2**, **3a** and polymorph I; type III in **3b** and polymorph II; and type IV in **4a**.

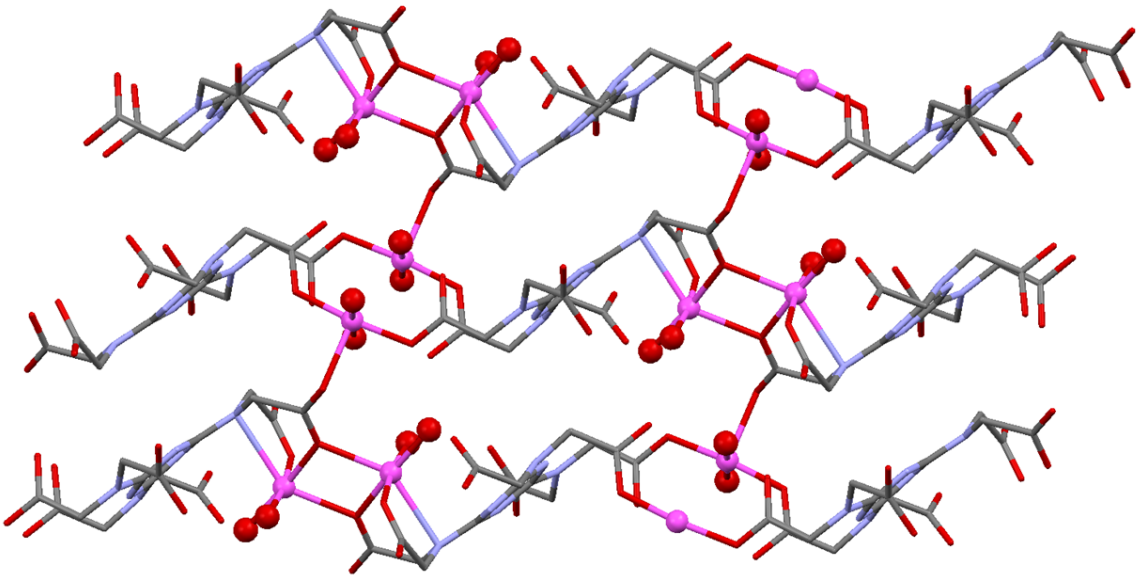


Figure S2. 2D metal-organic network in the reported TTHA-Cu based CP compositional variant,[10c] solid **3c**. The 2D aggregation of TTHA in both **3b** and **3c** are virtually identical (compare this with Figure 4). However, it may be noted that solid **3b** is a 2D CP, while the 2D sheets in solid **3c** are interlinked by square planar Cu units generating a 3D CP (not shown). Cu ions and water molecules are rendered as pink and red spheres, respectively.

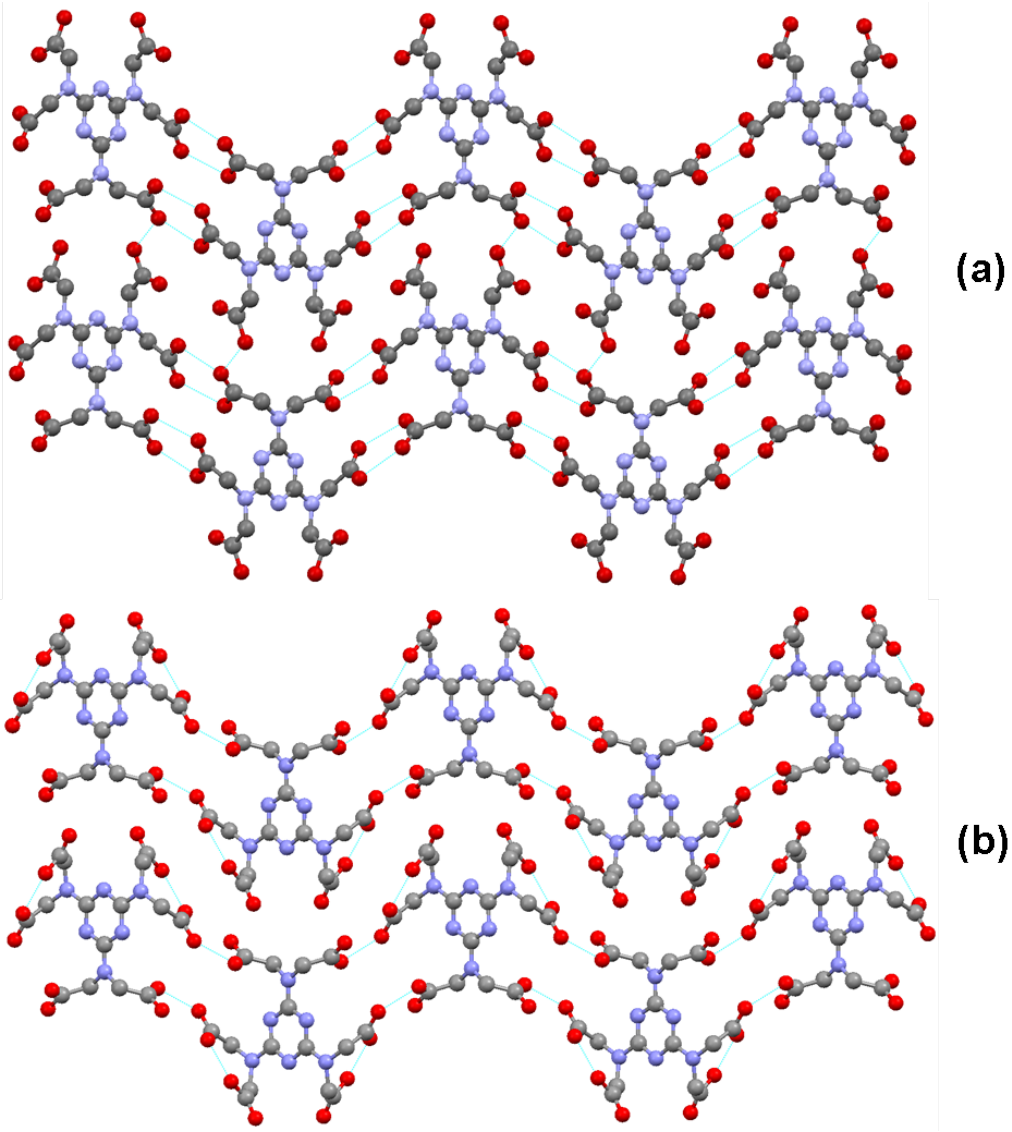


Figure S3. Packing diagrams of (a) TTHA form I and (b) TTHA form II. Solid **3a** (TTHA-Cu based CP) and TTHA polymorphs (I and II) have a virtually similar aggregation pattern (compare them with Figure 3). The 1D chains in TTHA form I and II are generated by hydrogen bond based synthons involving the two-point and single O-H···O contacts, respectively; while the 1D chains of solid **3a** are generated by the coordination bond based synthon I. Notice the similarities between the hydrogen bond and coordination bond based synthons.

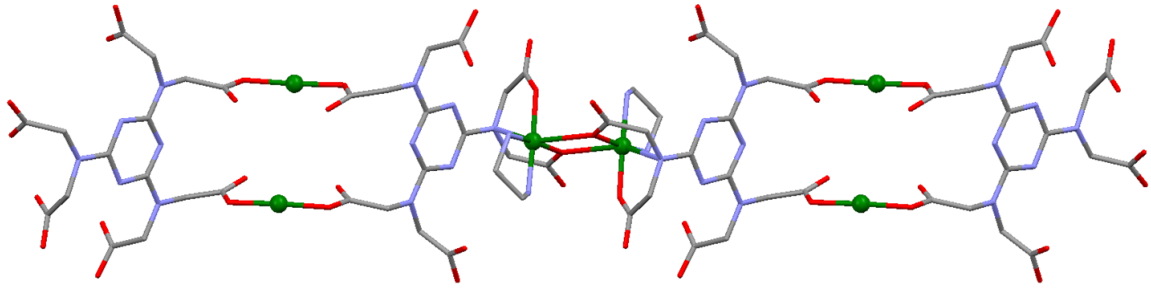


Figure S4. Synthons I and III in the 1D chains of TTHA-Cu-ethylenediamine based CP.[10c] Compare this with Figure 7c. Cu ions are rendered as green spheres.

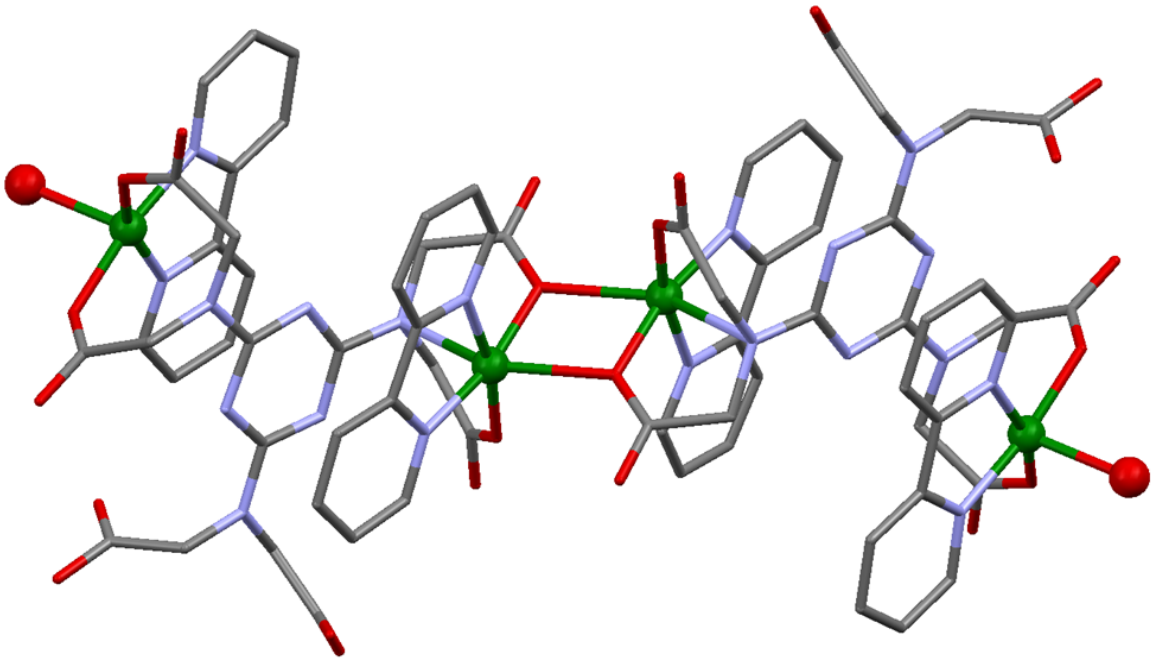
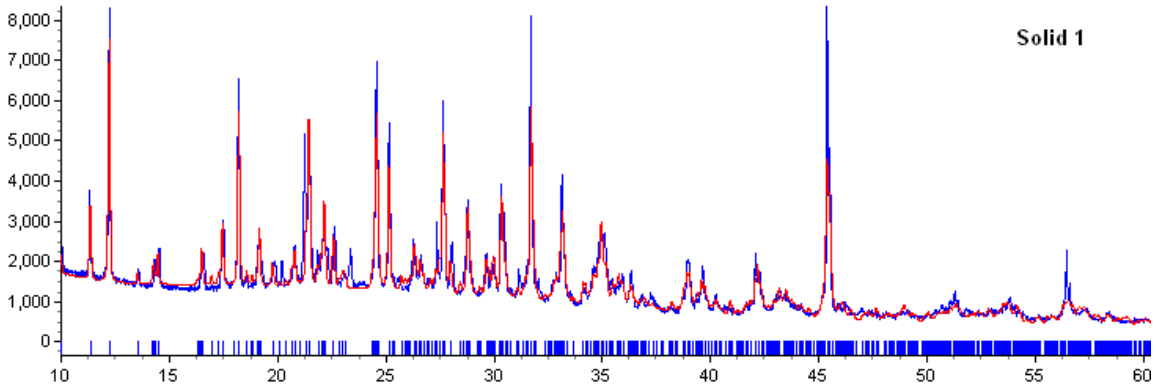
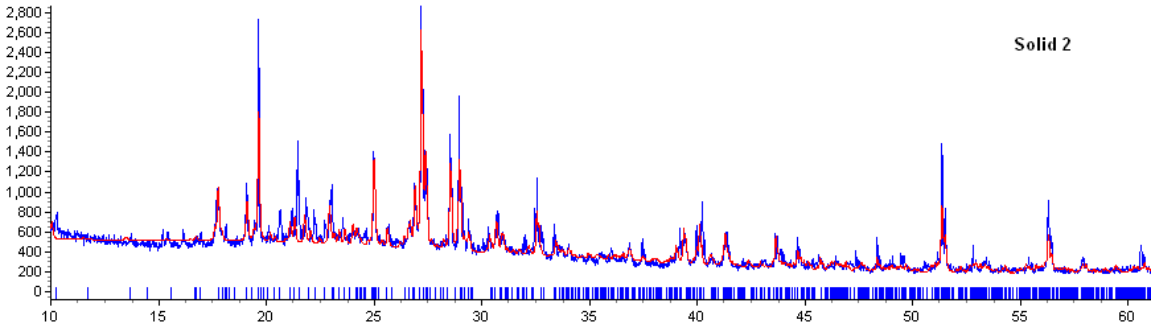
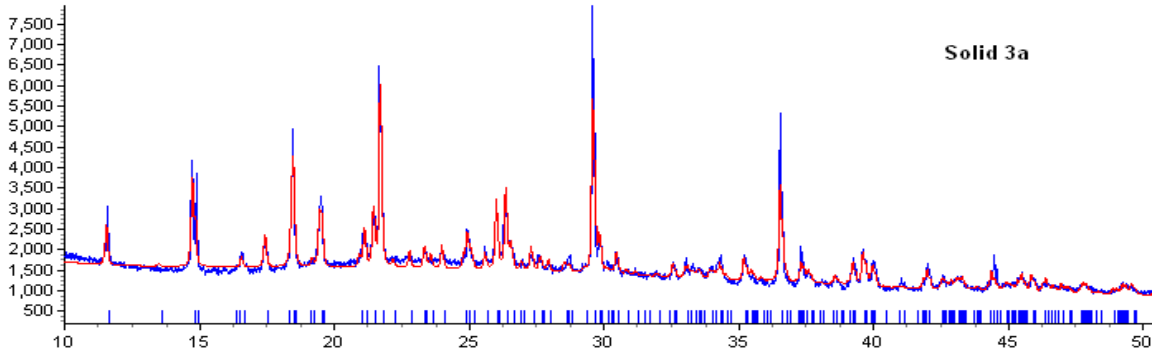


Figure S5. Synthon III in the molecular complex of TTHA-Cu-phenanthroline based CP.[10c] Cu ions and water molecules are rendered as green and red spheres, respectively.







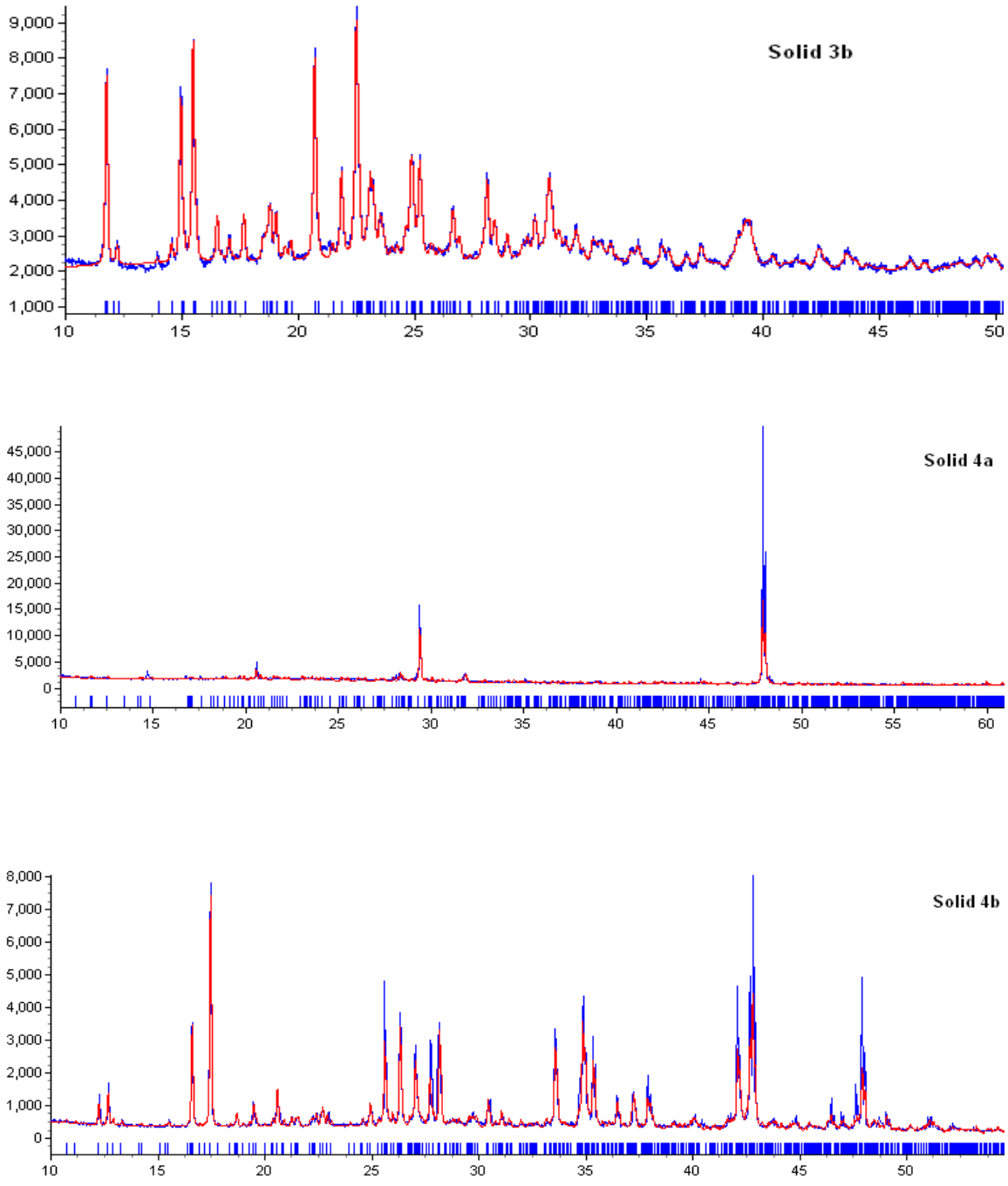


Figure S6. Rietveld analysis of powder XRDs confirming the monophasic nature of solids **1** through **4**.

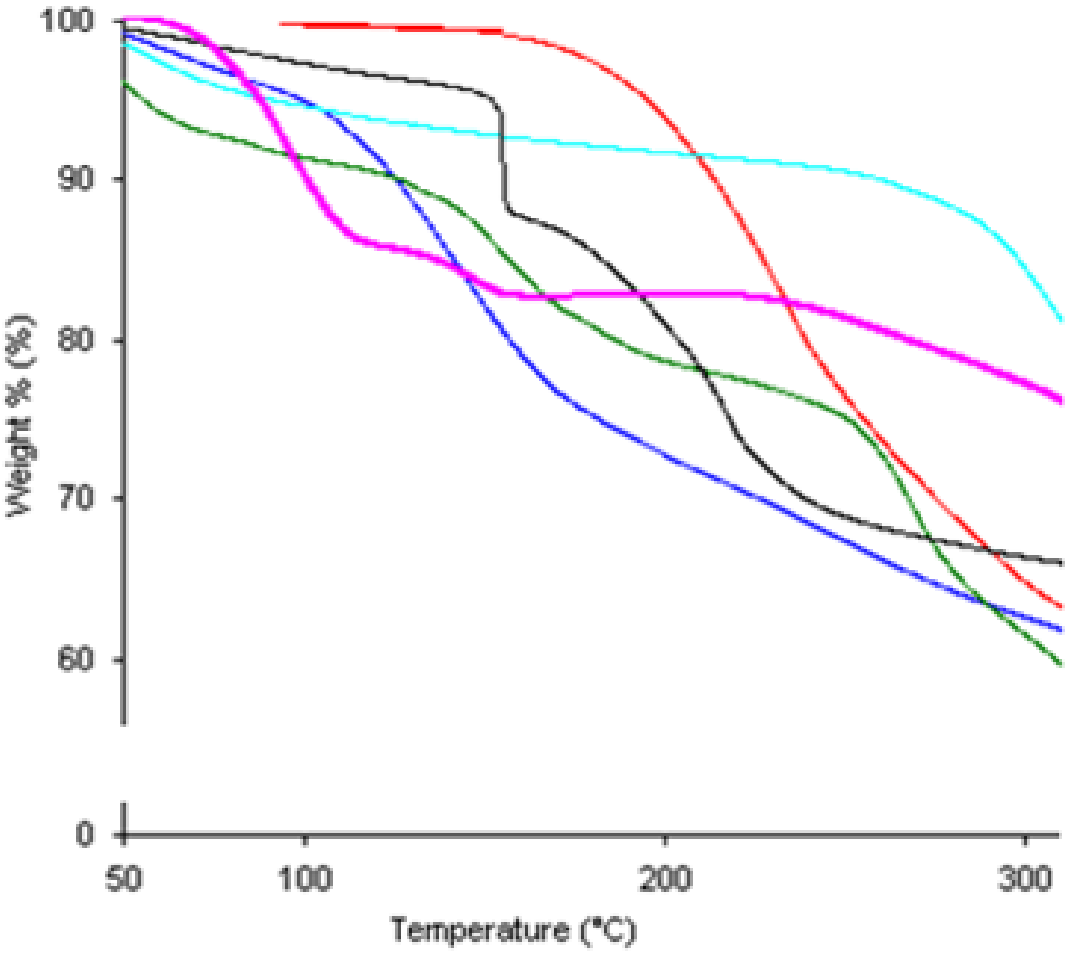


Figure S7. TGA thermograms of solids **1** through **4**.