

Fig. S1 (a) Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination, the as-synthesized and the desolvated products in compound **1**; and (b) Comparison of XRPD patterns of the simulated pattern from the single-crystal structure determination, the as-synthesized and the desolvated products in compound **2**.

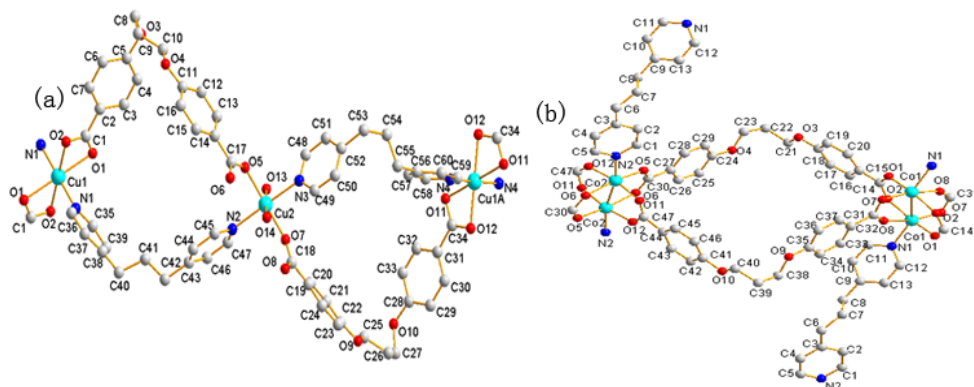


Fig. S2. (a) A view of the coordination environments at the three Cu^{II} centers in **1**(top); and (b) the coordination environments at the three Co^{II} centers in **2** (down).

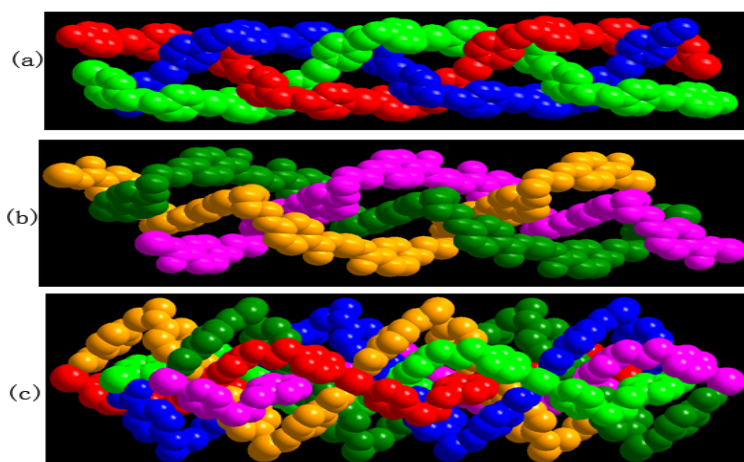


Fig. S3 (a) Space-filling view of the first type of triple-stranded molecular braid; (b) Space-filling view of the second type of triple-stranded molecular braid; and (c) Space-filling view of sextuple-stranded molecular braid along the *c* axis.

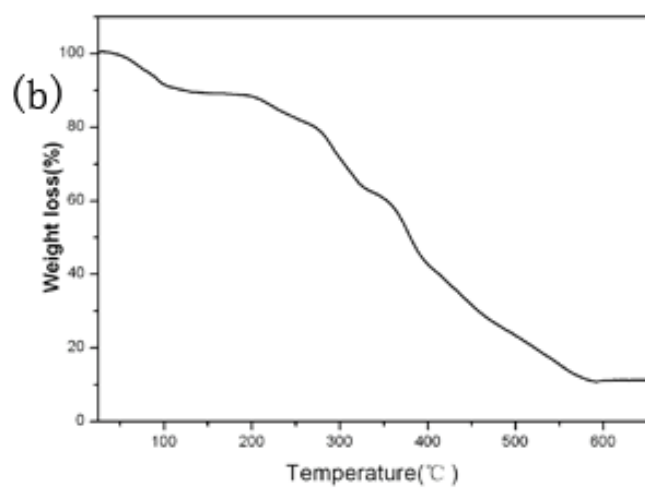
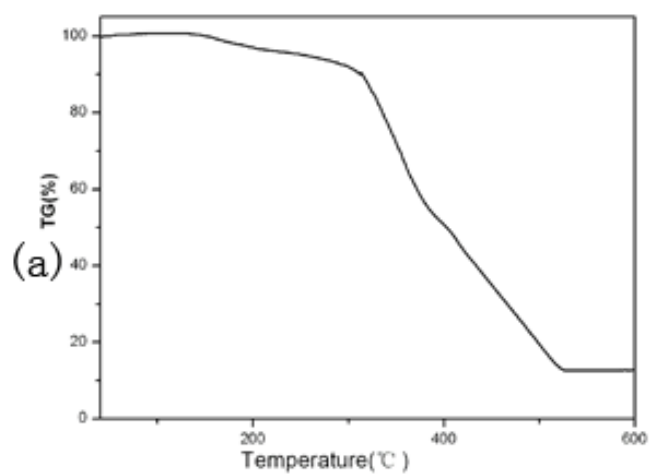


Fig. S4 (a) TG curve of compound 1; and (c) TG curve of compound 2.