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.