Electronic Supplementary Information

Ligand-deprotonation induced structural diversity in a ternary Cu^{II}-triazole-tetracarboxylate self-assembly system: synthesis, crystal structures, and magnetic behavior

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Table S1. Selected Hydrogen Bond Lengths (Å) and Angles (°) for **2 – 4**.

D–H···A	*d* (D–H)	*d* (H···A)	*d* (D···A)	∠DHA
2				
N8–H8'···O4[a]	0.90	2.35	3.110(1)	142
3				
O4–H4···O2[a]	0.82	1.91	2.675(2)	155
O5–H5···O3[b]	0.85	2.08	2.890(9)	160
N4–H4A···O2[c]	0.90	2.07	2.961(3)	171
N4–H4B···O1[d]	0.90	2.25	2.996(2)	140
4				
O4–H4···O5[a]	0.82	1.85	2.664(2)	171
O5–H5A···O2[b]	0.85	1.83	2.618(2)	154
O5–H5B···O3[c]	0.85	2.06	2.877(2)	162
N4–H4''···O2[d]	0.90	2.10	3.000(3)	175
N4–H4'···O1[e]	0.90	2.27	3.090(1)	150
N4–H4'···O5[f]	0.90	2.64	3.122(3)	114

Symmetry codes for **2**: [a] $x-1, 1/2-y, z+1$; for **3**: [a] $x, -y, z+1/2$; [b] $x, 1-y, z-1/2$; [c] $1-x, -y, 1-z$; [d] $1-x, 1-y, 1-z$; for **4**: [a] $x+1, y-1, z$; [b] $-x, 1-y, -z$; [c] $1-x, 1-y, -z$; [d] $x-1, y+1, z$; [e] $x-1, y, z$; [f] $x-1, y, z$.

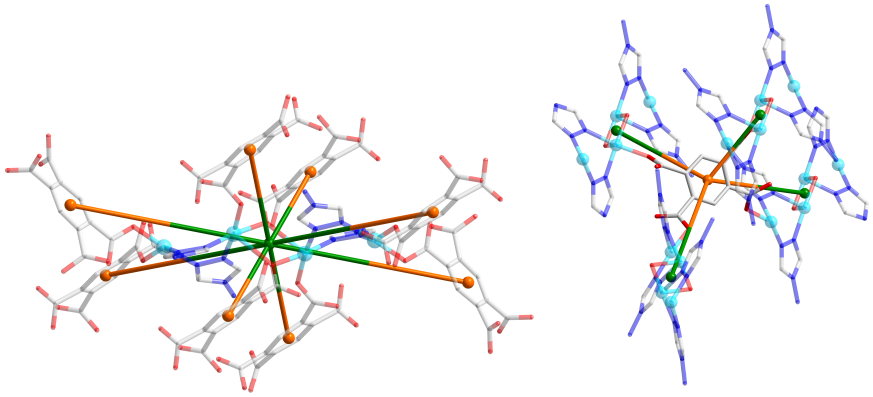

Fig. S1 The explanations for the 8-connected Cu^{II}_4 cluster and 4-connected $btec^{4-}$ in **1**.

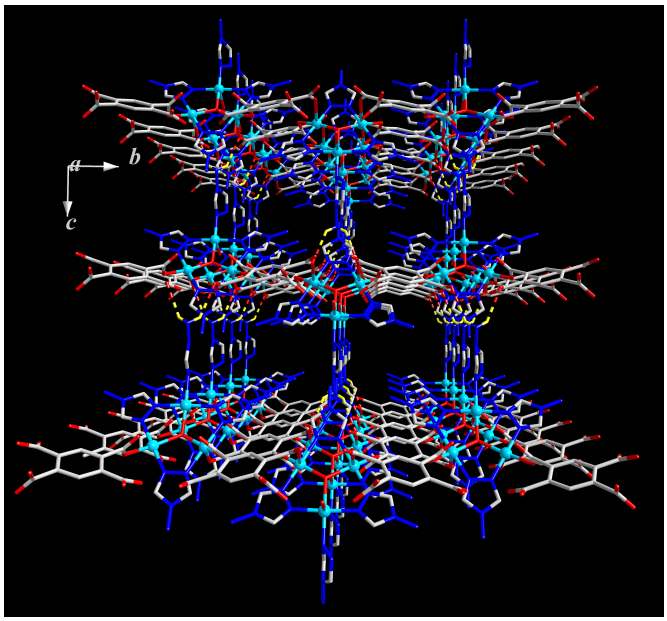

Fig. S2 3D supramolecular framework of **2** by N–H···O hydrogen-bonding interactions.

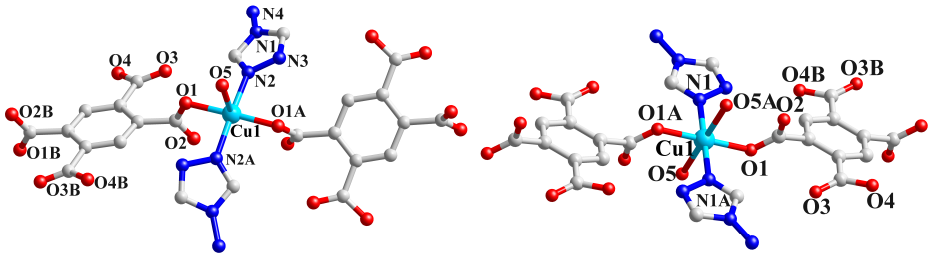

Fig. S3 Local coordination environment of Cu^{II} ion in **3** (left) and **4** (right) (H atom were omitted for clarity, Symmetric codes: A = 1 – *x*, *y*, 0.5 – *z*; B = *x* – 0.5, 0.5 – *y*, *z* – 0.5 for **3**, and A = – *x*, 1 – *y*, – *z*; B = 1 – *x*, – *y*, 1 – *z* for **4**).

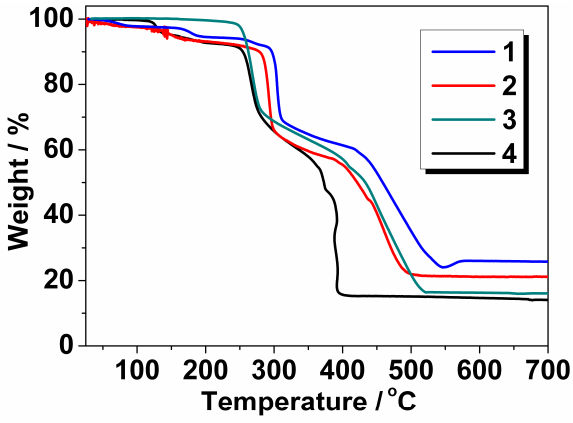

Fig. S4 TG curves for complexes **1 – 4**.

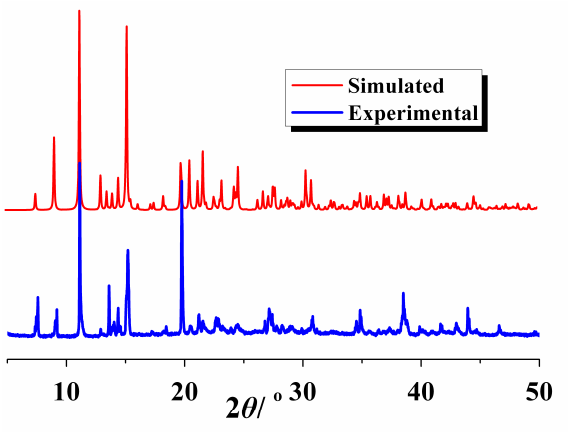

Fig. S5 X-ray powder diffraction patterns for **1**.

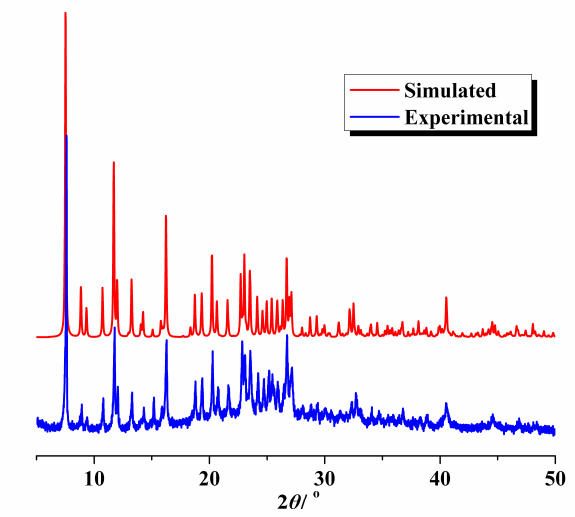

Fig. S6 X-ray powder diffraction patterns for **2**.

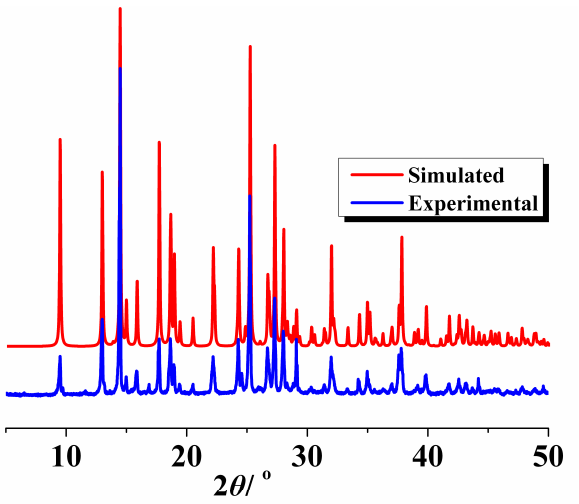

Fig. S7 X-ray powder diffraction patterns for **3**.

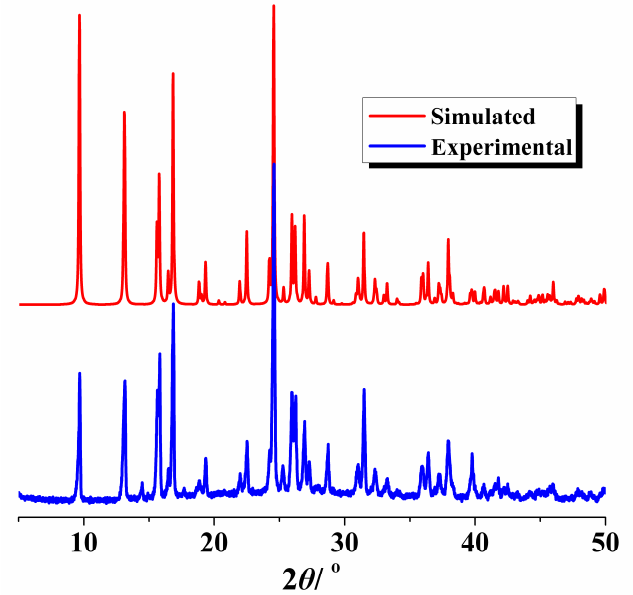

Fig. S8 X-ray powder diffraction patterns for **4**.

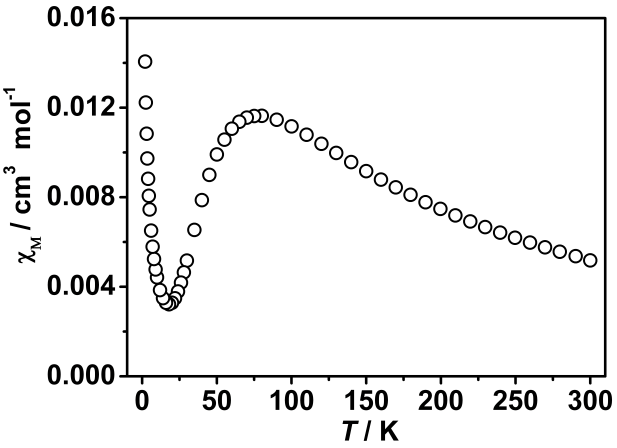

Fig. S9 Temperature dependence of χ_M for **1**.