Electronic Supplementary Information for

Distinct structures of coordination polymers incorporating flexible triazole-based ligand: topological diversities, crystal structures and property studies†

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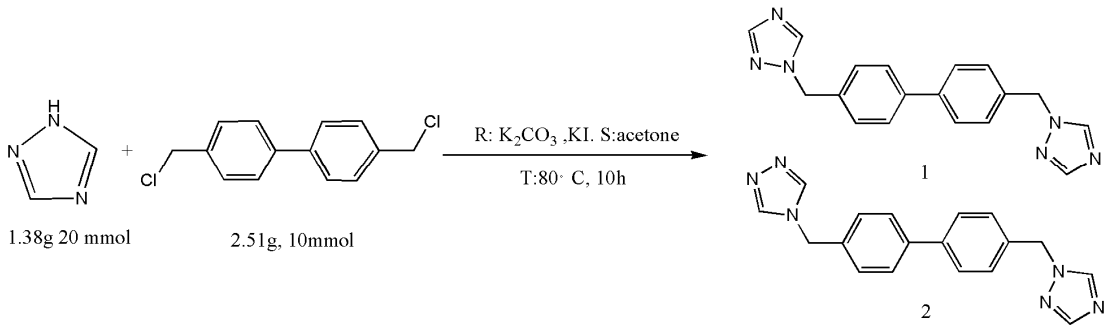
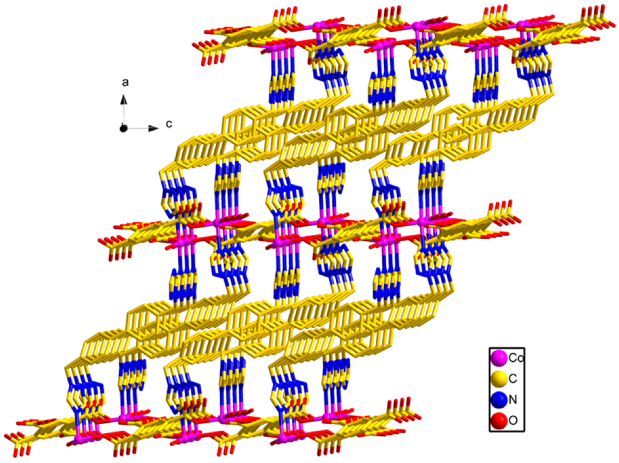
Note: Preparation of btmb ligand. The 4,4'-bis(1,2,4-triazol-1-ylmethyl)biphenyl (btmb) ligand was synthesized the same as literature methods,[1] yield: 63%. Mp: 168–170 °C. MS: m/z = 317.63 for $(Hbtmb)^+$. 1HNMR (CD_3OD): δ 5.468(4H), 7.393(2H), 7.634(2H), 8.008(2H), 8.608(2H). Anal. Calcd for $C_{18}H_{16}N_6$: C, 68.34; H, 5.100; N, 26.56. Found: C, 68.68; H, 5.13; N, 26.69. IR (KBr, cm^{-1}) for btmb: 3096(s), 1502(s), 1267(s), 139(s), 1016(s), 750(s).

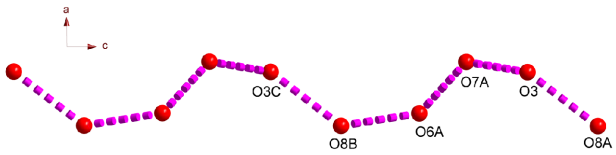
It is emphasized that the reaction may generate two kinds of product with the different positions of nitrogen atoms (1 and 2), however, it is difficult to separate and rationalize them. And the crystals containing 1 and 2 have also been obtained respectively.



[1] (a) X. R. Meng, Y. L. Song, H. W. Hou, H. Y. Han, B. Xiao, Y. T. Fan, and Y. Zhu, *Inorg. Chem.*, 2004, **43**, 3528; (b) X. L. Wang, C. Qin, E. B. Wang, Z. M. Su, *Chem. Commun.*, 2007, 4245.



(a)



(b)

Figure S1. (a). Perspective of the 3D framework of complex **2**. (b) 1D chain based on water clusters $(H_2O)_3$ in **2**. A: -x, -0.5+y, 0.5-z; B: -x, 1-y, -z; C: x, 0.5-y, -0.5+z.

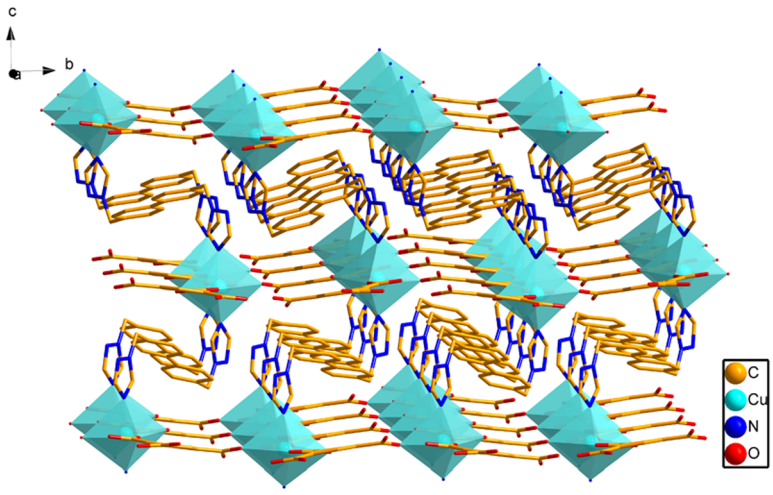


Figure S2. The 3D structure of complex **4**.

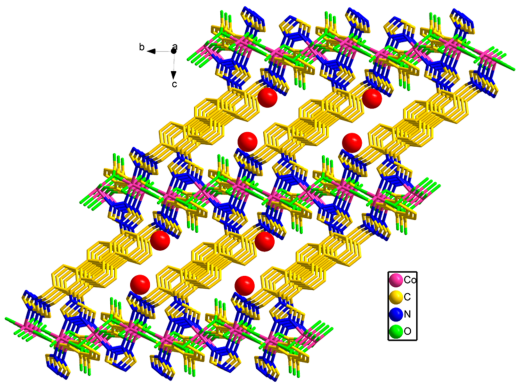


Figure S3. The 3D framework of complex **5**. red space filling model shows the channels with lattice water molecules.

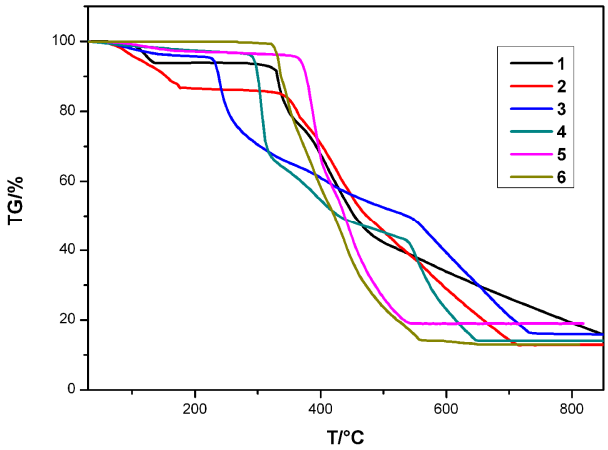
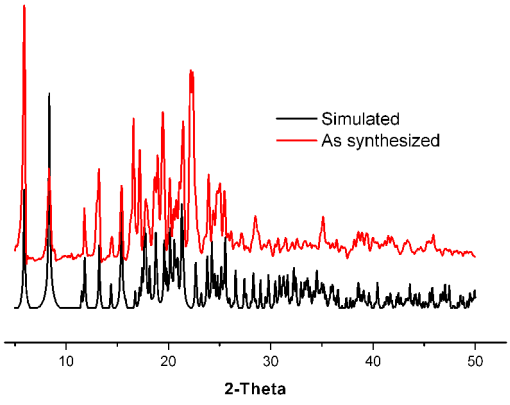
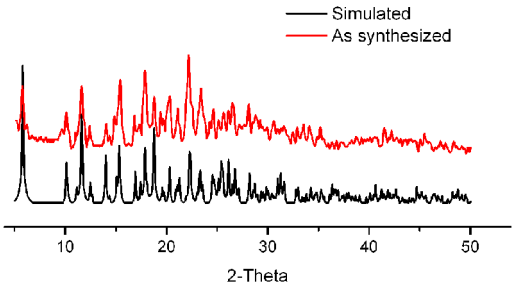


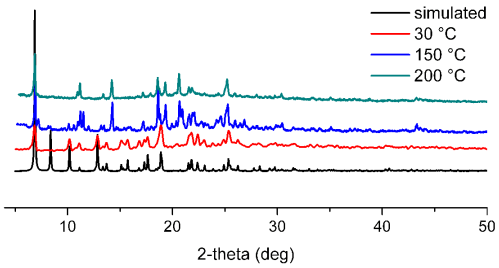
Figure S4. The TGA curves of complexes **1**–**6.**



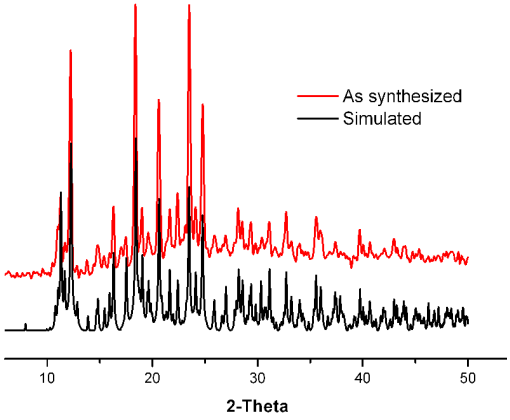
(a) Complex **1**.



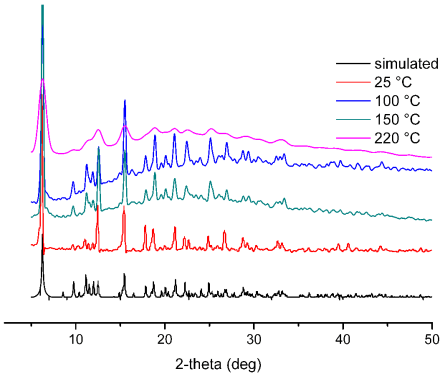
(b) Complex **2**.



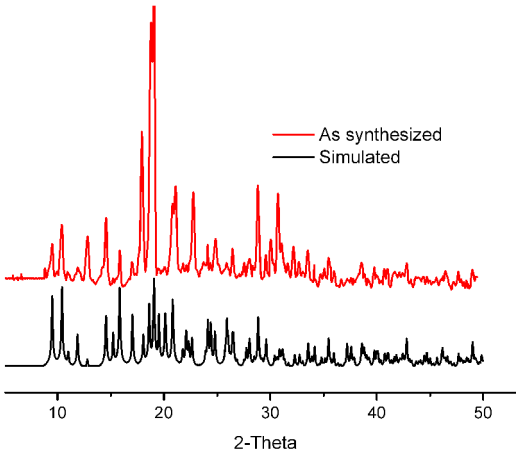
(c) Complex **3**.



(d) Complex **4**.



(e) Complex **5**.



(f) Complex **6**.

Figure S5. XRD of complexes **1**–**6.**

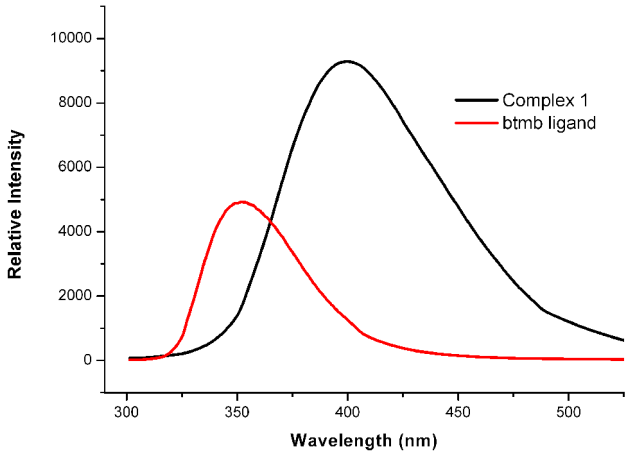
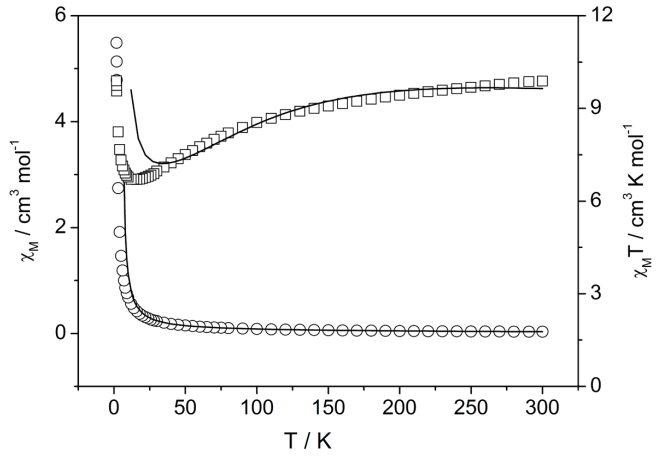
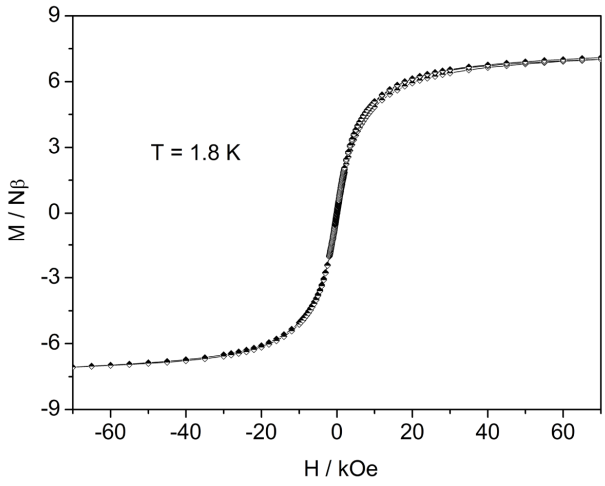


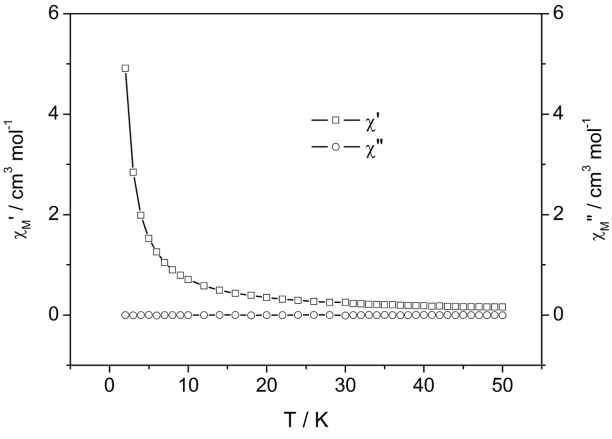
Figure S6. The solid-state photoluminescent spectra of complex **1** and the free btmb ligand at room temperature.



(a)



(b)



(c)

Figure S7. (a) Spin-orbit coupling fitting for **5**. (b) *M* vs H plots for **5**. (c) The AC magnetic susceptibility of complex **5**.

Table S1 Selected bond lengths [Å] and angles [°] for complexes **1**–**6**.

Complex 1					
Zn(1)–O(3)#1	1.931(6)	Zn(1)–O(1)	1.945(6)	Zn(1)–N(4)	2.007(7)
Zn(1)–N(1)	2.010(8)				
O(3)#1–Zn(1)–O(1)		98.0(3)	O(3)#1–Zn(1)–N(4)		123.6(3)
O(1)–Zn(1)–N(4)		106.5(3)	O(3)#1–Zn(1)–N(1)		107.7(3)
O(1)–Zn(1)–N(1)		115.6(3)	N(4)–Zn(1)–N(1)		105.9(3)
Complex 2					
Co(1)–O(4)#1	2.029(3)	Co(1)–O(5)	2.045(4)	Co(1)–N(1)	2.098(4)
Co(1)–N(4)#2	2.143(4)	Co(1)–O(2)	2.173(3)	Co(1)–O(1)	2.189(3)
O(4)#1–Co(1)–O(5)		111.98(14)	O(5)–Co(1)–O(2)		157.18(14)
O(4)#1–Co(1)–N(1)		97.05(14)	N(1)–Co(1)–O(2)		87.08(15)
O(5)–Co(1)–N(1)		88.37(15)	N(4)#2–Co(1)–O(2)		95.82(14)
O(4)#1–Co(1)–N(4)#2		85.70(14)	O(4)#1–Co(1)–O(1)		149.08(12)
O(5)–Co(1)–N(4)#2		87.89(15)	O(5)–Co(1)–O(1)		97.89(14)
N(1)–Co(1)–N(4)#2		175.99(15)	N(1)–Co(1)–O(1)		91.40(14)
O(4)#1–Co(1)–O(2)		90.77(12)	N(4)#2–Co(1)–O(1)		87.69(14)
O(2)–Co(1)–O(1)		59.91(11)			
Complex 3					
Cu(1)–O(3)	1.953(3)	Cu(1)–N(1)	1.980(5)	Cu(1)–O(2) #1	2.626(8)
Cu(1)–O(1)#1	1.978(4)	Cu(1)–N(4)#2	2.000(5)	Cu(1) –O5	2.799(5)
O(3)–Cu(1)–O(1)#1		165.09(17)	O(3)–Cu(1)–N(4)#2		92.58(16)
O(3)–Cu(1)–N(1)		89.86(16)	O(1)#1–Cu(1)–N(4)#2		91.01(18)
O(1)#1–Cu(1)–N(1)		89.29(18)	N(1)–Cu(1)–N(4)#2		169.24(19)
Complex 4					
Cu(1)–O(2)	1.966(2)	Cu(1)–O(4)#1	1.972(2)	Cu(1)–N(4)	1.973(3)
Cu(1)–N(1)	1.980(3)	Cu(1)–O(6)#2	2.372(2)	Cu(1)–O(3)	2.732(1)
O(2) –Cu(1)–O(4)#1		156.21(10)	N(4)–Cu(1)–N(1)		178.26(11)
O(2)–Cu(1)–N(4)		92.03(11)	O(2)–Cu(1)–O(6)#2		107.27(9)
O(4)#1–Cu(1)–N(4)		90.64(11)	O(4)#1–Cu(1)–O(6)#2		96.29(8)
O(2)–Cu(1)–N(1)		88.00(11)	N(4)–Cu(1)–O(6)#2		91.32(10)
O(4)#1–Cu(1)–N(1)		90.03(11)	N(1)–Cu(1)–O(6)#2		87.01(10)
Complex 5					
Co(1)–O(1)	2.049(4)	Co(1)–O(3)	2.164(4)	Co(2)–O(3)#5	2.139(4)

Co(1)–O(2)#1	2.058(4)	Co(1)–N(1)	2.175(6)	Co(2)–O(3)#6	2.139(4)
Co(1)–O(5)#2	2.064(4)	Co(2)–O(6)	2.048(4)	Co(2)–N(5)#7	2.150(5)
Co(1)–N(4)#3	2.130(5)	Co(2)–O(6)#4	2.048(4)	Co(2)–N(5)#8	2.150(5)
O(1)–Co(1)–O(2)#1		93.87(17)	O(6)–Co(2)–O(6)#4		180.0
O(1)–Co(1)–O(5)#2		174.13(17)	O(6)–Co(2)–O(3)#5		95.66(16)
O(2)#1–Co(1)–O(5)#2		89.52(17)	O(6)#4–Co(2)–O(3)#5		84.34(16)
O(1)–Co(1)–N(4)#3		97.80(19)	O(6)–Co(2)–O(3)#6		84.34(16)
O(2)#1–Co(1)–N(4)#3		95.35(19)	O(6)#4–Co(2)–O(3)#6		95.66(16)
O(5)#2–Co(1)–N(4)#3		86.64(19)	O(3)#5–Co(2)–O(3)#6		180.0
O(1)–Co(1)–O(3)		84.00(16)	O(6)–Co(2)–N(5)#7		81.15(18)
O(2)#1–Co(1)–O(3)		177.87(16)	O(6)#4–Co(2)–N(5)#7		98.85(18)
O(5)#2–Co(1)–O(3)		92.62(16)	O(3)#5–Co(2)–N(5)#7		86.86(18)
N(4)#3–Co(1)–O(3)		84.81(18)	O(3)#6–Co(2)–N(5)#7		93.14(18)
O(1)–Co(1)–N(1)		90.4(2)	O(6)–Co(2)–N(5)#8		98.85(18)
O(2)#1–Co(1)–N(1)		86.8(2)	O(6)#4–Co(2)–N(5)#8		81.15(18)
O(5)#2–Co(1)–N(1)		85.0(2)	O(3)#5–Co(2)–N(5)#8		93.14(18)
N(4)#3–Co(1)–N(1)		171.4(2)	O(3)#6–Co(2)–N(5)#8		86.86(18)
O(3)–Co(1)–N(1)		93.30(19)	N(5)#7–Co(2)–N(5)#8		180.0
Complex 6					
Co(1)–O(5)	1.909(5)	Co(1)–N(1)	2.037(5)	Co(1)–N(1)#2	2.037(5)
Co(1)–O(1)#1	1.976(4)				
O(5)–Co(1)–O(1)#1		110.9(2)	O(5)–Co(1)–N(1)#2		104.58(15)
O(5)–Co(1)–N(1)		104.58(15)	O(1)#1–Co(1)–N(1)#2		112.69(14)
O(1)#1–Co(1)–N(1)		112.69(14)	N(1)–Co(1)–N(1)#2		110.8(3)
C(1)–O(1)–Co(1)#3		108.0(4)			

[a] Symmetry codes: For 1: #1 x, -y+1/2, z+1/2. For 2: #1 -x, y-1/2, -z+1/2; #2 x-1, -y+1/2, z-1/2. For 3: #1 -x+1/2, y-1/2, -z+1/2; #2 -x, y-1, -z+1/2. For 4: #1 x+1, y, z; #2 –x+1, y-1/2, -z+1/2. For 5: #1 -x+1, -y+2, -z+1; #2 x+1, y, z; #3 x-1, y+1, z+1; #4 -x-1, -y+3, -z+1; #5 -x, -y+3, -z+1; #6 x-1, y, z; #7 -x+1, -y+2, -z; #8 x-2, y+1, z+1. For 6: #1 x, y, z+1; #2 x, -y+1/2, z; #3 x, y, z-1.