Ligand-Directed and pH-Controlled Assembly of Chiral 3d-3d Heterometallic Metal-Organic Frameworks

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Table S1 Hydrogen bonding distances (Å) and angles (°) for complex **1**

D–H ··· A	*d*(D-H)	*d*(H···A)	*d*(D ···A)	∠(D – H ··· A)
C2-H1····O16	0.9500	2.3900	3.339(16)	175
C13-H6····O2#1	0.9500	2.3000	2.963(15)	126
C31-H7····O10#2	0.9500	2.3700	3.178(15)	142
C51-H10····O4#1	0.9500	2.5200	3.231(14)	131
C53-H12····O8#2	0.9500	2.3900	2.979(15)	120
C104-H14····O7#3	0.9500	2.5700	3.479(12)	159
C111-H15····O1	0.9500	2.2100	3.159(14)	173
C113-H17····O2#4	0.9500	2.5300	3.458(14)	165
C131-H18····O7	0.9500	2.2200	3.162(11)	171
C133-H20····O8#3	0.9500	2.4400	3.364(12)	166
C205-H22····O17#5	0.9500	2.5300	3.36(2)	146
C305-H25····O13#6	0.9500	2.5500	3.427(17)	153

Symmetry transformations used to generate equivalent atoms: #1 1-y, 1+x-y, z; #2 1+x-y, x, -1/2+z; #3 1-x+y, 2-x, z; #4 -x+y, 1-x, z; #5 1-y, x-y, z; #6 y, -x+y, 1/2+z.

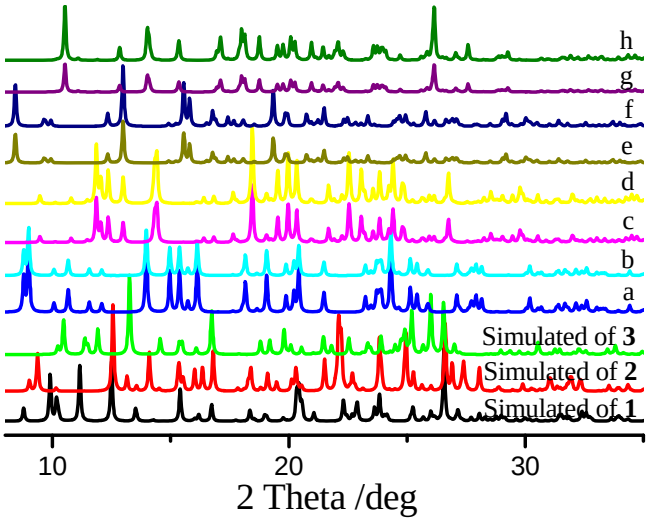

Figure S1. PXRD patterns of simulated of complexes **1-3**, products of $ZnCl_2$ with tib, 1,2,4-H_3BTC under pH values of 8 ~ 9 (a) and 5 ~ 6 (b), products of $CoCl_2 \cdot 6H_2O$ with tib, 1,2,4-H_3BTC under pH values of 8 ~ 9 (c) and 5 ~ 6 (d), products of $ZnCl_2$ with tib, 1,3,5-H_3BTC under pH values of 8 ~ 9 (e) and 5 ~ 6 (f), products of $CoCl_2 \cdot 6H_2O$ with tib, 1,3,5-H_3BTC under pH values of 8 ~ 9 (g) and 5 ~ 6 (h), respectively.

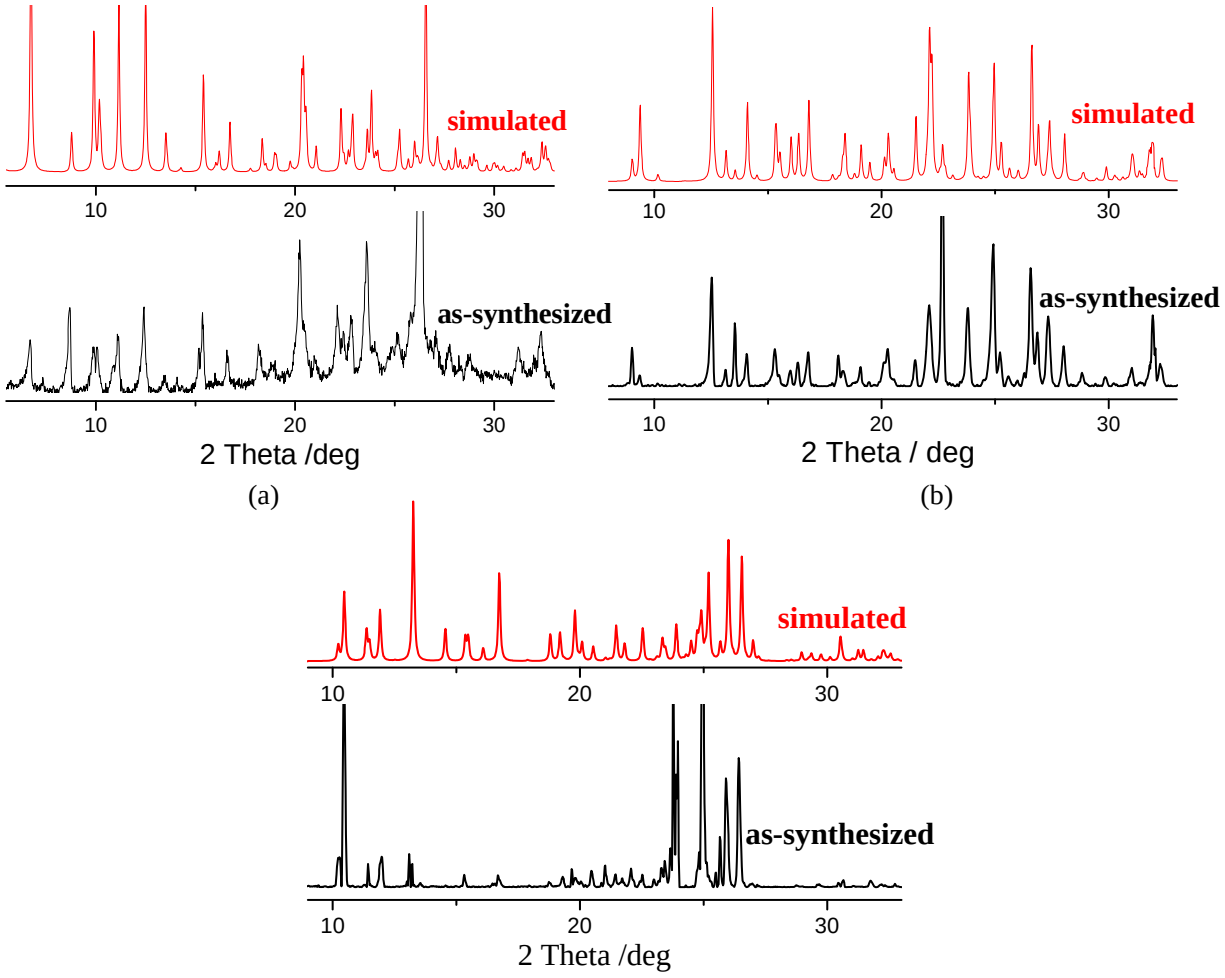

Figure S2. The PXRD patterns for complexes **1** (a), **2** (b) and **3** (c).

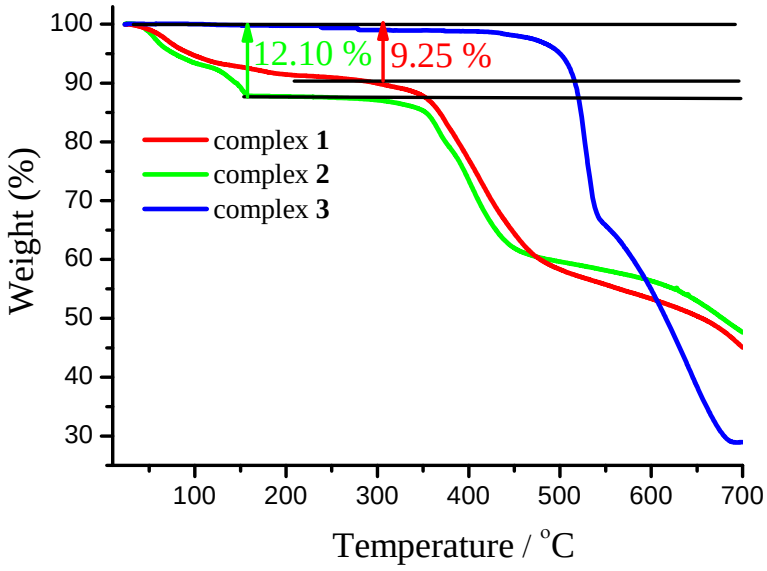

Figure S3. The TG curves of complexes **1**, **2** and **3**.

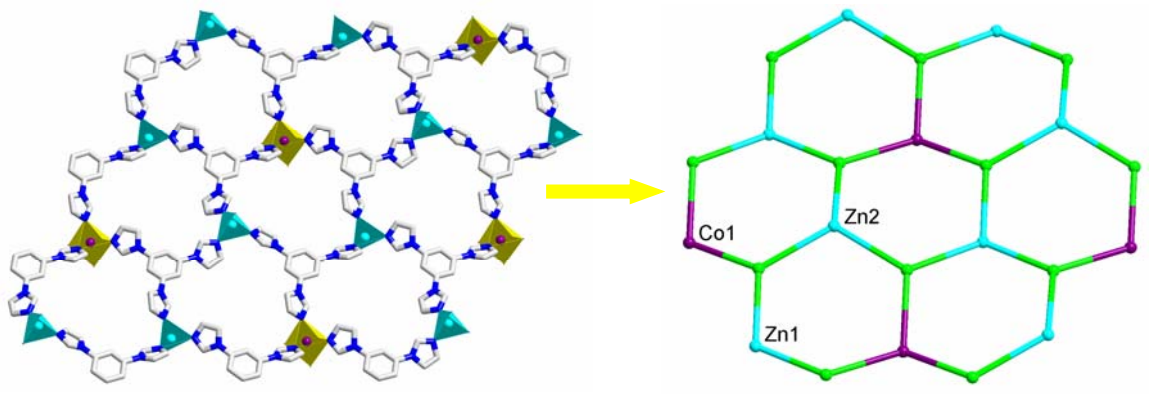

Figure S4. The polyhedral and topological view of 2D $[Zn_2Co(tib)_3(H_2O)_5]^{6+}$ part in **1**.

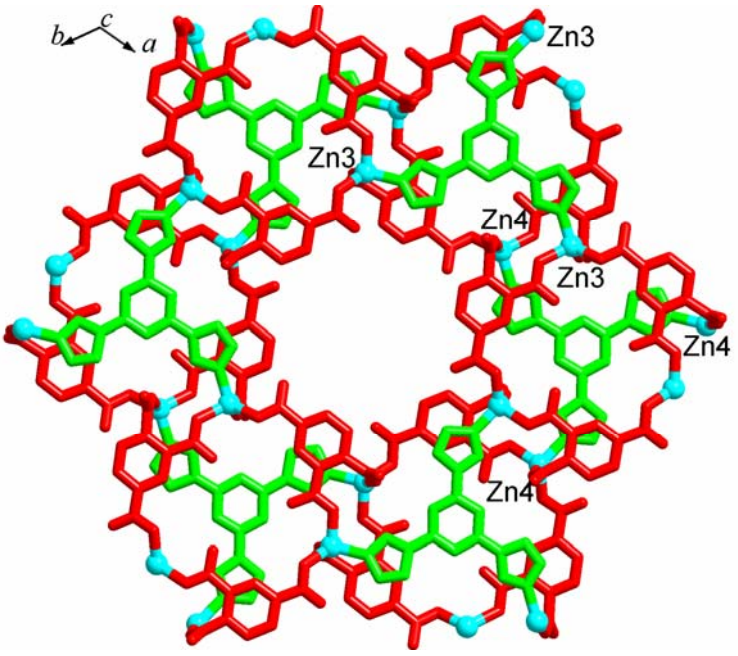

Figure S5. The 2D network of $[Zn_6(tib)_2(BTC)_6]^{6-}$ part in **1**.

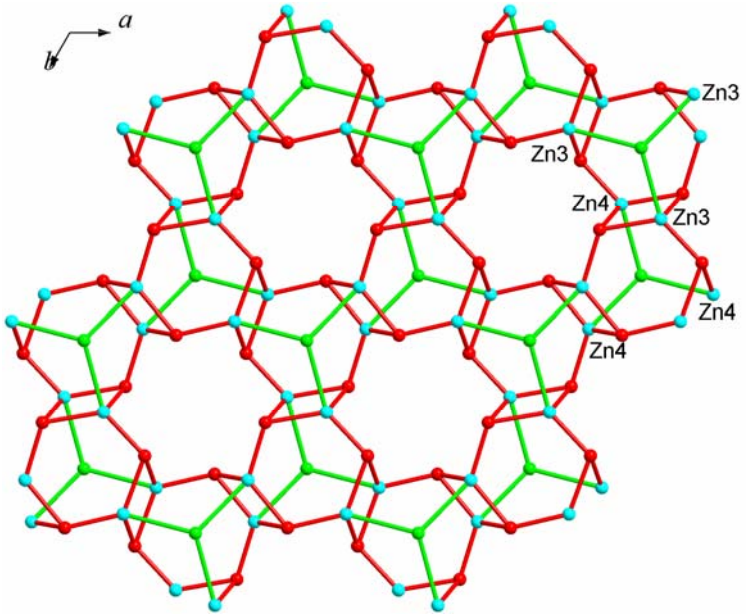

Figure S6. The topological view of 2D $[Zn_6(tib)_2(BTC)_6]^{6-}$ part in **1**.

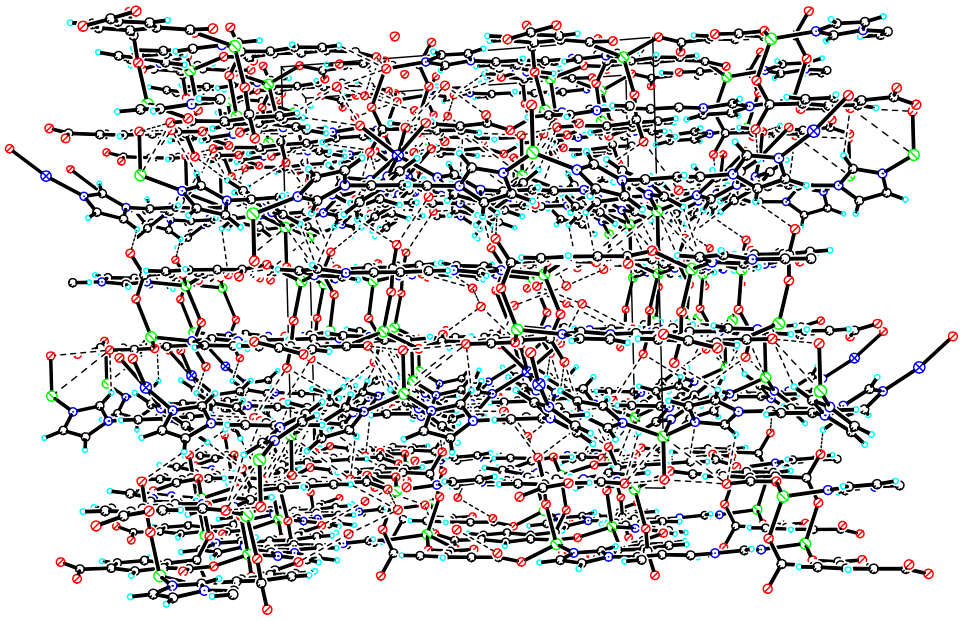

Figure S7. The 3D framework of **1**.

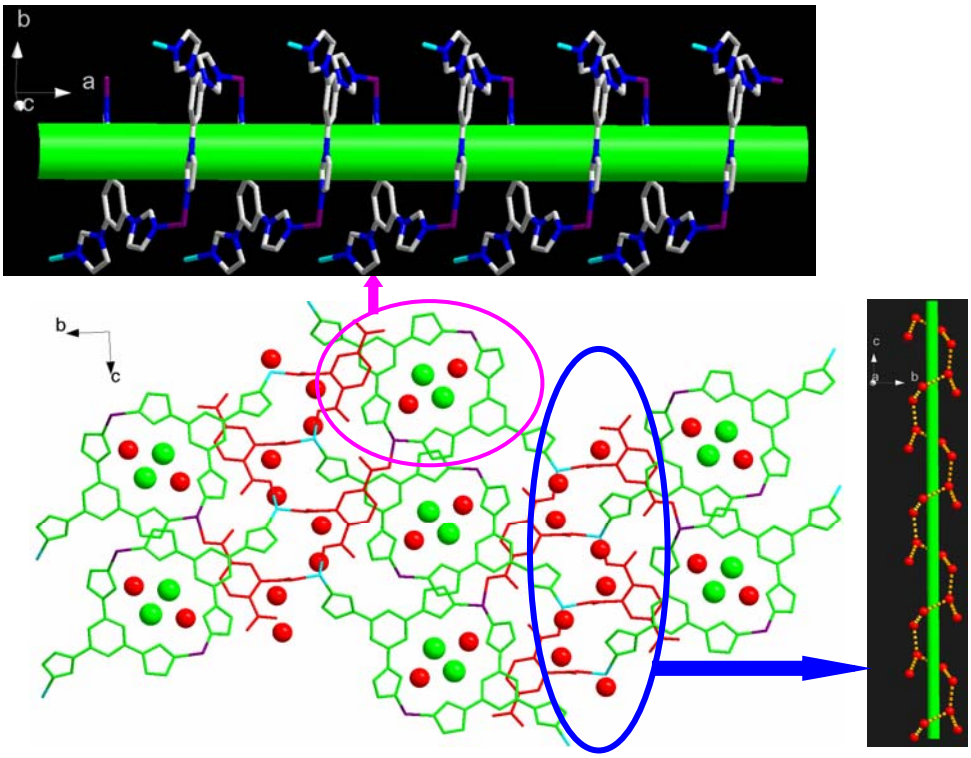

Figure S8. The 3D framework of **2** and the helical chains along *a* (up), and *c* (right) directions, respectively.

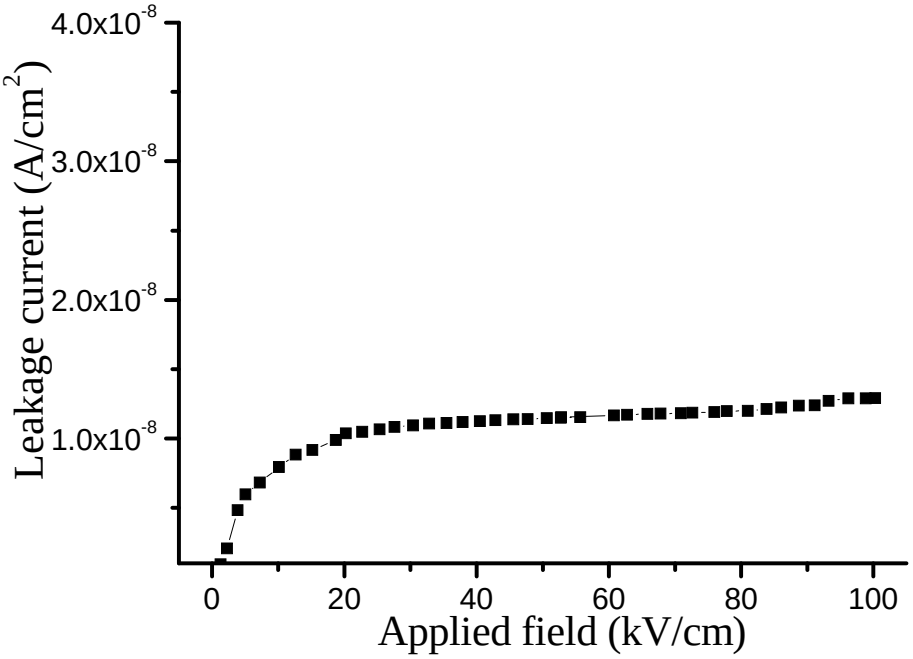

Figure S9. Plot of leakage current vs. applied field for **1**.