Electronic Supplementary Information

Solvent-mediated assembly of chiral/achiral hydrophilic Ca(II)–tetrafluoroterephthalate coordination frameworks: 3D chiral water aggregation, structural transformation and selective CO_2 adsorption

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Table S1. The selected bond distances (Å) and angles (deg) for complexes **1**–**3** [a]

		Complex **1**			
Ca1–O1	2.335(3)	Ca1–O1#2	2.335(3)	Ca1–O2	2.556(3)
Ca1–O2#2	2.556(3)	Ca1–O2#3	2.419(3)	Ca1–O2#4	2.419(3)
Ca1–O1WB	2.280(1)				
O1–Ca1–O1 WB	106.4(7)	O1WB–Ca1–O1#2	92.5(6)	O1WB–Ca1–O2	142.2(6)
O1WB–Ca1–O2#2	161.1(9)	O1WB–Ca1–O2#3	92.5(7)	O1WB–Ca1–O2#4	74.4(7)
O1–Ca1–O1#2	160.9(1)	O1–Ca1–O2	80.73(9)	O1–Ca1–O2#2	82.04(9)
O1–Ca1–O2#3	81.22(9)	O1–Ca1–O2#4	101.00(9)	O2–Ca1–O2#2	50.8(1)
O2–Ca1–O2#3	121.39(8)	O2–Ca1–O2#4	71.8(1)	O2#3–Ca1–O2#4	166.8(2)
		Complex **2**			
Ca1–O1	2.457(4)	Ca1–O1#2	2.457(4)	Ca1–O2#1	2.745(4)
Ca1–O3	2.377(4)	Ca1–O3#2	2.377(4)	Ca1–O3#3	2.338(5)
O1–Ca1–O1#2	80.2(1)	O1–Ca1–O2#1	123.3(1)	O1–Ca1–O2#3	82.1(1)
O1–Ca1–O3	87.1(1)	O1–Ca1–O3#2	146.6(1)	O2#1–Ca1–O2#3	148.9(1)
O2#1–Ca1–O3	79.4(1)	O2#1–Ca1–O3#2	84.8(1)	O3–Ca1–O3#2	118.3(1)
		Complex **3**			
Ca1–O1	2.599(1)	Ca1–O1#1	2.599(1)	Ca1–O3	2.431(2)
Ca1–O4	2.60(1)	Ca1–O4#1	2.59(1)	Ca1–O4#2	2.557(1)
Ca1–O4#4	2.557(1)	Ca1–O5	2.449(2)	Ca1–O5#3	2.468(1)
O1–Ca1–O1#1	123.38(6)	O1–Ca1–O3	118.27(2)	O1–Ca1–O4	67.75(4)
O1–Ca1–O4#1	133.73(5)	O1–Ca1–O4#2	133.05(5)	O1–Ca1–O4#4	66.34(4)
O1–Ca1–O5	71.45(4)	O1–Ca1–O5#3	72.70(3)	O3–Ca1–O4	72.80(5)
O3–Ca1–O4#2	70.72(5)	O3–Ca1–O5	129.46(6)	O3–Ca1–O5#3	131.49(6)
O4–Ca1–O4#1	74.83(6)	O4–Ca1–O4#2	143.50(6)	O4–Ca1–O4#4	93.20(5)
O4–Ca1–O5	139.21(3)	O4–Ca1–O5#3	69.13(5)	O4#2–Ca1–O4#4	76.00(6)
O4#4–Ca1–O5	69.97(5)	O5–Ca1–O5#3	99.05(7)		

[a] Symmetry transformations used to generate equivalent atoms: For **1**, #2: $x, y, -z+2$; #3: $-x+1, -y+1, z+1/2$; #4: $-x+1, -y+1, -z+3/2$; For **2**, #1: $-x+1, -y+1, -z$; #2: $-x+1, y, -z+1/2$; #3: $x, -y+1, z+1/2$; For **3**, #1: $x, -y+3/2, z$; #2: $x+1, -y+3/2, z$; #3: $x-1, y, z$; #4: $x+1, y, z$.

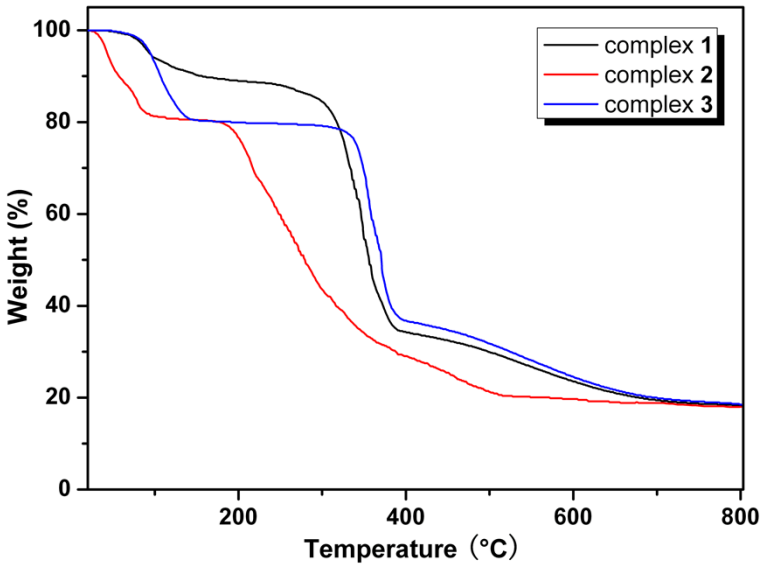

Fig. S1 TGA curves of complexes **1**–**3**.

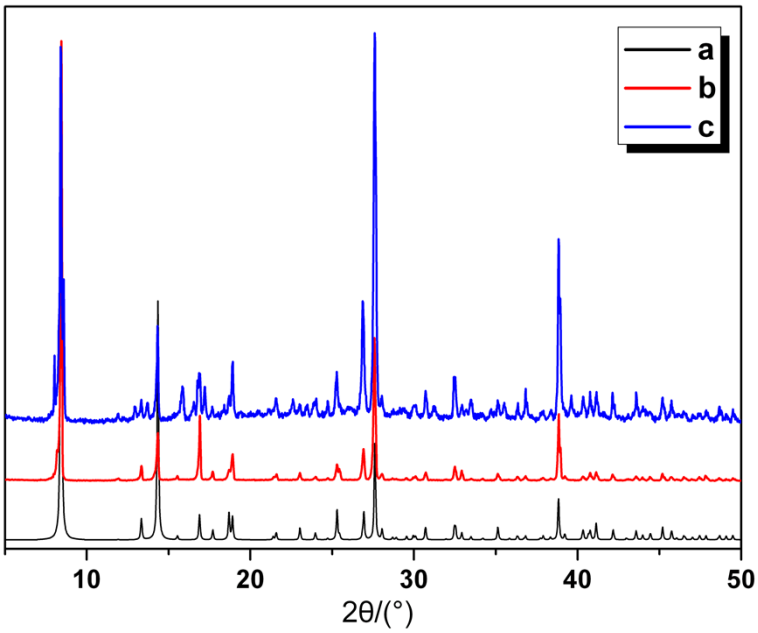

Fig. S2 XRPD patterns for: (a) **1** as simulated from the single-crystal data; (b) as-synthesized **1**; and (c) prepared by dehydrating **1** at 160 °C for 6 h.

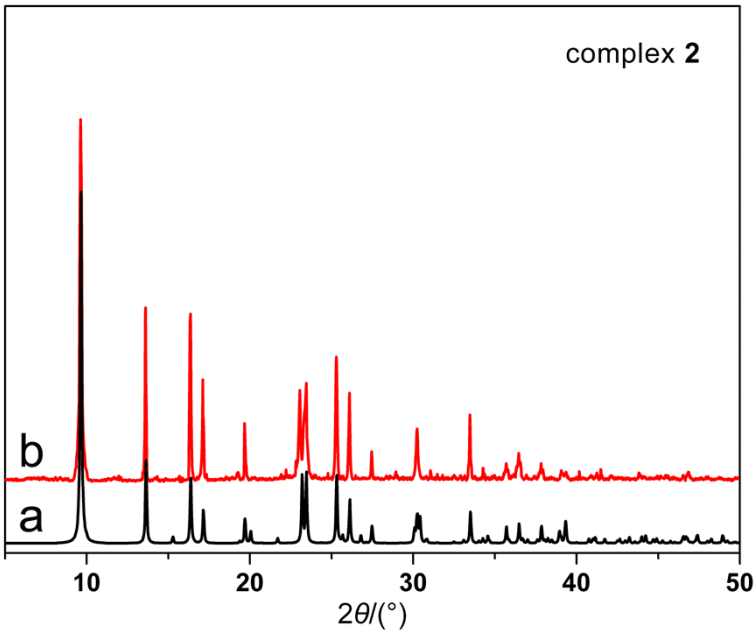

Fig. S3 XRPD patterns for: (a) **2** as simulated from the single-crystal data; (b) as-synthesized **2**.

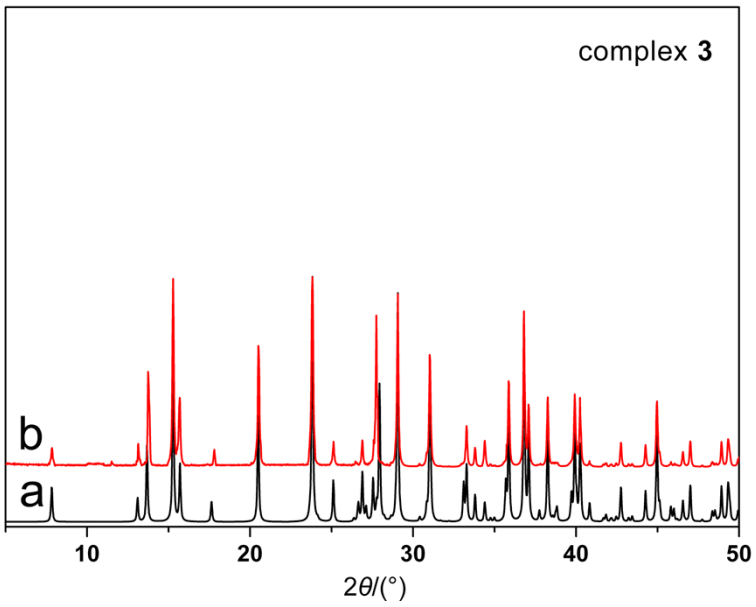

Fig. S4 XRPD patterns for: (a) **3** as simulated from the single-crystal data; (b) as-synthesized **3**.