Supporting information

Structure Versatility of Coordination Polymers Constructed from a New Semirigid Polycarboxylate Ligand and Polynuclear Metal Clusters

De-Liang Yang,[a] Xin Zhang,[a] Yuan-Gen Yao,[a] * and Jian Zhang [a]

[a]Key Laboratory of Coal to Ethylene Glycol and Its Related Technology, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China

E-mail: yyg@fjirsm.ac.cn; Fax: +86-591-8371-4946; Tel: +86-591-8371-1523

Table S1 Selected bond lengths (Å) and angles (°) for **1−5**[a].

	Compound 1		
Cd(1)-O(1W)	2.210(5)	Cd(1)-O(6)#1	2.246(4)
Cd(1)-O(2)	2.333(4)	Cd(1)-O(13)	2.405(5)
Cd(1)-O(7)#1	2.484(5)	Cd(1)-O(1)	2.492(5)
Cd(1)-O(4)b	2.591(3)	Cd(2)-O(7)a	2.234(3)
Cd(1)-O(12)	2.494(5)	Cd(2)-O(18)#2	2.205(5)
Cd(2)-O(9)#3	2.290(5)	Cd(2)-O(11)	2.348(5)
Cd(2)-O(10)	2.464(4)	Cd(2)-O(4)	2.486(5)
Cd(2)-O(3)	2.512(6)	Cd(2)-O(17)#2	2.540(5)
Cd(3)-O(8)#3	2.155(5)	Cd(3)-O(12)	2.225(4)
Cd(3)-O(16)#4	2.264(5)	Cd(3)-O(2)	2.265(5)
Cd(3)-O(4)	2.276(5)	Cd(3)-O(10)	2.374(4)
O(1W)-Cd(1)-O(6)#1	98.79(19)	O(1W)-Cd(1)-O(2)	96.35(18)
O(6)#1-Cd(1)-O(2)	159.80(17)	O(1W)-Cd(1)-O(13)	89.1(2)
O(6)#1-Cd(1)-O(13)	99.90(17)	O(2)-Cd(1)-O(13)	93.62(15)
O(1W)-Cd(1)-O(7)#1	143.4(2)	O(6)#1-Cd(1)-O(7)#1	54.63(16)
O(2)-Cd(1)-O(7)#1	105.70(15)	O(13)-Cd(1)-O(7)#1	117.62(18)
O(1W)-Cd(1)-O(1)	83.7(2)	O(6)#1-Cd(1)-O(1)	114.69(17)
O(2)-Cd(1)-O(1)	53.88(15)	O(13)-Cd(1)-O(1)	145.33(15)
O(7)#1-Cd(1)-O(1)	86.15(16)	O(1W)-Cd(1)-O(12)	139.3(2)
O(6)#1-Cd(1)-O(12)	100.57(16)	O(2)-Cd(1)-O(12)	75.92(14)
O(13)-Cd(1)-O(12)	52.51(16)	O(7)#1-Cd(1)-O(12)	75.46(16)
O(1)-Cd(1)-O(12)	118.95(15)	O(18)#2-Cd(2)-O(9)#3	96.58(18)
O(18)#2-Cd(2)-O(11)	119.51(19)	O(9)#3-Cd(2)-O(11)	86.96(18)

O(18)#2-Cd(2)-O(10)	159.38(18)	O(9)#3-Cd(2)-O(10)	102.37(15)
O(11)-Cd(2)-O(10)	54.34(15)	O(18)#2-Cd(2)-O(4)	111.78(18)
O(9)#3-Cd(2)-O(4)	81.72(17)	O(11)-Cd(2)-O(4)	128.38(15)
O(10)-Cd(2)-O(4)	79.27(14)	O(18)#2-Cd(2)-O(3)	95.79(19)
O(9)#3-Cd(2)-O(3)	133.50(17)	O(11)-Cd(2)-O(3)	124.00(18)
O(10)-Cd(2)-O(3)	77.00(15)	O(4)-Cd(2)-O(3)	52.13(16)
O(18)#2-Cd(2)-O(17)#2	54.31(18)	O(9)#3-Cd(2)-O(17)#2	144.42(17)
O(11)-Cd(2)-O(17)#2	90.93(17)	O(10)-Cd(2)-O(17)#2	105.07(15)
O(4)-Cd(2)-O(17)#2	125.30(17)	O(3)-Cd(2)-O(17)#2	75.30(17)
O(8)#3-Cd(3)-O(12)	100.90(17)	O(8)#3-Cd(3)-O(16)#4	95.0(2)
O(12)-Cd(3)-O(16)#4	99.16(17)	O(8)#3-Cd(3)-O(2)	171.29(17)
O(12)-Cd(3)-O(2)	82.89(16)	O(16)#4-Cd(3)-O(2)	92.07(18)
O(8)#3-Cd(3)-O(4)	92.50(17)	O(12)-Cd(3)-O(4)	159.32(18)
O(16)#4-Cd(3)-O(4)	95.23(19)	O(2)-Cd(3)-O(4)	81.82(16)
O(8)#3-Cd(3)-O(10)	86.63(18)	O(12)-Cd(3)-O(10)	79.70(15)
O(16)#4-Cd(3)-O(10)	178.15(18)	O(2)-Cd(3)-O(10)	86.35(16)
O(4)-Cd(3)-O(10)	85.50(17)		

Compound 2

Cd(1)-O(1)	2.202(3)	Cd(1)-O(7)#1	2.242(3)
Cd(1)-O(4)#2	2.245(3)	Cd(1)-O(8)#3	2.301(3)
Cd(1)-O(9)#3	2.458(3)	Cd(1)-O(3)#2	2.736(3)
Cd(1)-O(6)#1	2.807(3)	Ca(1)-O(11)	2.285(3)
Ca(1)-O(6)#1	2.289(3)	Ca(1)-O(10)	2.330(4)
Ca(1)-O(3)#4	2.333(3)	Ca(1)-O(2)	2.345(3)
Ca(1)-O(9)#3	2.419(3)	O(1)-Cd(1)-O(7)#1	102.22(12)
O(1)-Cd(1)-O(4)#2	107.33(11)	O(7)#1-Cd(1)-O(4)#2	84.63(12)
O(1)-Cd(1)-O(8)#3	100.82(12)	O(7)#1-Cd(1)-O(8)#3	156.55(12)
O(4)#2-Cd(1)-O(8)#3	92.68(12)	O(1)-Cd(1)-O(9)#3	112.99(10)
O(7)#1-Cd(1)-O(9)#3	110.74(11)	O(4)#2-Cd(1)-O(9)#3	131.73(10)
O(8)#3-Cd(1)-O(9)#3	55.13(10)	O(1)-Cd(1)-O(6)#1	89.92(10)
O(7)#1-Cd(1)-O(6)#1	50.19(11)	O(8)#3-Cd(1)-O(6)#1	125.82(11)
O(4)#2-Cd(1)-O(6)#1	134.48(9)	O(9)#3-Cd(1)-O(6)#1	71.67(10)
O(3)#2-Cd(1)-O(6)#1	106.68(9)	O(1)-Cd(1)-O(3)#2	159.08(10)
O(7)#1-Cd(1)-O(3)#2	80.04(11)	O(4)#2-Cd(1)-O(3)#2	51.88(9)
O(8)#3-Cd(1)-O(3)#2	80.03(10)	O(9)#3-Cd(1)-O(3)#2	84.87(9)
O(11)-Ca(1)-O(6)#1	174.86(15)	O(11)-Ca(1)-O(10)	95.44(16)
O(2)-Ca(1)-O(9)#3	89.58(14)	O(11)-Ca(1)-O(3)#4	88.13(13)
O(6)#1-Ca(1)-O(3)#4	92.49(12)	O(10)-Ca(1)-O(3)#4	95.47(13)
O(11)-Ca(1)-O(2)	93.79(13)	O(6)#1-Ca(1)-O(2)	85.67 (12)
O(10)-Ca(1)-O(2)	83.55(13)	O(3)#4-Ca(1)-O(2)	177.92(12)
O(11)-Ca(1)-O(9)#3	92.68(14)	O(6)#1-Ca(1)-O(9)#3	82.19(11)
O(10)-Ca(1)-O(9)#3	163.18(12)	O(3)#4-Ca(1)-O(9)#3	99.50(11)
O(2)-Ca(1)-O(9)#3	81.23(11)		

Compound 3

Cd(1)-O(1)	2.239(3)	Cd(1)-O(4)#1	2.268(2)
Cd(1)-O(7)#2	2.354(2)	Cd(1)-O(9)#3	2.375(3)
Cd(1)-O(6)#2	2.380(2)	Cd(1)-O(8)#3	2.454(3)
Cd(1)-O(5)#1	2.711(2)	Ca(1)-O(1W)	2.388(3)
Ca(1)-O(5)#1	2.334(3)	Ca(1)-O(9)	2.352(3)
Ca(1)-O(10)	2.352(3)	Ca(1)-O(2W)	2.420(3)
Ca(1)-O(2)#3	2.325(3)	O(7)#2-Cd(1)-O(6)#2	54.45(9)
O(1)-Cd(1)-O(4)#1	103.52(10)	O(9)#3-Cd(1)-O(6)#2	103.86(9)
O(1)-Cd(1)-O(7)#2	119.55(11)	O(1)-Cd(1)-O(8)#3	137.81(9)
O(4)#1-Cd(1)-O(7)#2	77.27(9)	O(4)#1-Cd(1)-O(8)#3	87.81(11)
O(4)#1-Cd(1)-O(6)#2	86.70(10)	O(6)#2-Cd(1)-O(8)#3	109.37(10)
O(4)#1-Cd(1)-O(9)#3	122.55(9)	O(9)#3-Cd(1)-O(8)#3	54.25(9)
O(7)#2-Cd(1)-O(9)#3	144.26(10)	O(7)#2-Cd(1)-O(8)#3	102.52(10)
O(1)-Cd(1)-O(6)#2	93.69(10)	O(1)-Cd(1)-O(5)#1	75.74(9)
O(1)-Cd(1)-O(9)#3	130.84(9)	O(4)#1-Cd(1)-O(5)#1	51.50(7)
O(7)#2-Cd(1)-O(5)#1	128.69(7)	O(9)#3-Cd(1)-O(5)#1	78.44(7)
O(8)#3-Cd(1)-O(5)#1	80.72(9)	O(6)#2-Cd(1)-O(5)#1	169.12(7)
O(2)#3-Ca(1)-O(5)#1	81.03(10)	O(10)-Ca(1)-O(1W)	83.81(13)
O(2)#3-Ca(1)-O(10)	115.77(12)	O(9)-Ca(1)-O(1W)	105.79(11)
O(5)#1-Ca(1)-O(10)	155.94(11)	O(2)#3-Ca(1)-O(2W)	83.33(11)
O(2)#3-Ca(1)-O(9)	79.32(9)	O(5)#1-Ca(1)-O(2W)	95.15(10)
O(5)#1-Ca(1)-O(1W)	80.25(12)	O(10)-Ca(1)-O(2W)	71.36(12)
O(10)-Ca(1)-O(9)	80.30(11)	O(9)-Ca(1)-O(2W)	135.84(11)
O(2)#3-Ca(1)-O(1W)	160.41(11)	O(1W)-Ca(1)-O(2W)	104.04(12)
O(5)#1-Ca(1)-O(9)	121.37(9)		

Compound 4

Ba(1)-O(10)#1	2.731(3)	Ba(1)-O(21)	2.763(3)
Ba(1)-O(20)#2	2.779(3)	Ba(1)-O(16)	2.799(3)
Ba(1)-O(6)#3	2.809(3)	Ba(1)-O(17)	2.843(3)
Ba(1)-O(3)#4	2.853(3)	Ba(1)-O(2W)	2.880(3)
Ba(1)-O(17)#2	3.069(3)	Ba(2)-O(18)#2	2.722(3)
Ba(2)-O(12)	2.743(3)	Ba(2)-O(2)#5	2.749(3)
Ba(2)-O(9)	2.759(3)	Ba(2)-O(2W)#2	2.781(3)
Ba(2)-O(1W)	2.834(3)	Ba(2)-O(16)	3.006(3)
Ba(2)-O(20)	3.038(3)	Ba(2)-O(17)#2	3.046(3)
O(10)#1-Ba(1)-O(21)	132.81(11)	O(6)#3-Ba(1)-O(3)#4	101.61(9)
O(10)#1-Ba(1)-O(20)#2	131.67(9)	O(17)-Ba(1)-O(3)#4	127.57(9)
O(21)-Ba(1)-O(20)#2	88.82(10)	O(20)#2-Ba(1)-O(2W)	65.09(9)
O(10)#1-Ba(1)-O(16)	78.14(9)	O(21)-Ba(1)-O(2W)	131.06(9)

O(21)-Ba(1)-O(16)	102.64(9)	O(10)#1-Ba(1)-O(2W)	68.64(8)
O(20)#2-Ba(1)-O(16)	121.45(8)	O(6)#3-Ba(1)-O(2W)	126.27(8)
O(10)#1-Ba(1)-O(6)#3	68.32(10)	O(16)-Ba(1)-O(2W)	125.63(9)
O(21)-Ba(1)-O(6)#3	69.22(11)	O(16)-Ba(1)-O(2W)	69.91(8)
O(20)#2-Ba(1)-O(6)#3	158.03(9)	O(10)#1-Ba(1)-O(17)#2	66.49(9)
O(16)-Ba(1)-O(6)#3	66.33(8)	O(21)-Ba(1)-O(17)#2	138.35(9)
O(10)#1-Ba(1)-O(17)	80.63(10)	O(20)#2-Ba(1)-O(17)#2	75.57(10)
O(21)-Ba(1)-O(17)	143.77(10)	O(16)-Ba(1)-O(17)#2	63.64(8)
O(20)#2-Ba(1)-O(17)	71.08(8)	O(6)#3-Ba(1)-O(17)#2	109.08(9)
O(16)-Ba(1)-O(17)	66.45(8)	O(17)-Ba(1)-O(17)#2	68.56(10)
O(6)#3-Ba(1)-O(17)	66.99(8)	O(3)#4-Ba(1)-O(17)#2	115.68(8)
O(10)#1-Ba(1)-O(3)#4	105.16(10)	O(2W)-Ba(1)-O(17)#2	124.14(8)
O(21)-Ba(1)-O(3)#4	64.73(10)	O(20)#2-Ba(1)-O(3)#4	64.37(8)
O(16)-Ba(1)-O(3)#4	127.42(8)	O(18)#2-Ba(2)-O(12)	152.48(9)
O(9)-Ba(2)-O(1W)	66.40(10)	O(18)#2-Ba(2)-O(2)#5	138.74(10)
O(2W)#2-Ba(2)-O(1W)	142.54(10)	O(12)-Ba(2)-O(2)#5	68.73(8)
O(18)#2-Ba(2)-O(16)	104.84(9)	O(18)#2-Ba(2)-O(9)	99.91(9)
O(12)-Ba(2)-O(16)	69.13(8)	O(12)-Ba(2)-O(9)	67.02(9)
O(2)#5-Ba(2)-O(16)	92.05(8)	O(2)#5-Ba(2)-O(9)	99.70(9)
O(9)-Ba(2)-O(16)	126.13(8)	O(18)#2-Ba(2)-O(2W)#2	68.42(9)
O(2W)#2-Ba(2)-O(16)	104.54(8)	O(12)-Ba(2)-O(2W)#2	138.84(8)
O(1W)-Ba(2)-O(16)	74.60(9)	O(2)#5-Ba(2)-O(2W)#2	71.00(9)
O(18)#2-Ba(2)-O(20)	106.09(9)	O(9)-Ba(2)-O(2W)#2	129.07(9)
O(12)-Ba(2)-O(20)	87.68(8)	O(18)#2-Ba(2)-O(1W)	75.57(10)
O(2)#5-Ba(2)-O(20)	62.66(8)	O(12)-Ba(2)-O(1W)	76.96(9
O(16)-Ba(2)-O(20)	42.65(7)	O(2)#5-Ba(2)-O(1W)	145.68(10)
O(2W)#2-Ba(2)-O(20)	66.34(8)	O(18)#2-Ba(2)-O(17)#2	45.09(8)
O(1W)-Ba(2)-O(20)	116.31(9)	O(12)-Ba(2)-O(17)#2	129.98(8)
O(9)-Ba(2)-O(20)	153.71(8)	O(2W)#2-Ba(2)-O(17)#2	68.30(8)
O(1W)-Ba(2)-O(17)#2	79.22(9)	O(9)-Ba(2)-O(17)#2	137.22(8)
O(20)-Ba(2)-O(17)#2	64.98(7)	O(2)#5-Ba(2)-O(17)#2	122.78(8)
O(16)-Ba(2)-O(17)#2	62.37(8)		

Compound 5

Ba(1)-O(2)#1	2.733(4)	Ba(1)-O(19)	2.749(5)
Ba(1)-O(13)#2	2.782(4)	Ba(1)-O(12)	2.793(4)
Ba(1)-O(8)#3	2.814(4)	Ba(1)-O(2W)	2.824(4)
Ba(1)-O(7)#4	2.861(5)	Ba(1)-O(11)	2.880(5)
Ba(1)-O(11)#2	3.061(4)	Ba(2)-O(10)	2.725(4)
Ba(2)-O(4)	2.740(4)	Ba(2)-O(1)	2.741(4)
Ba(2)-O(16)#5	2.745(4)	Ba(2)-O(11)	2.774(4)
Ba(2)-O(1W)	2.840(5)	Ba(2)-O(12)#2	3.005(4)
Ba(2)-O(13)#2	3.006(4)	Ba(2)-O(2W)	3.055(4)
O(2)#1-Ba(1)-O(19)	134.05(16)	O(13)#2-Ba(1)-O(11)	71.10(12)

O(2)#1-Ba(1)-O(13)#2	132.78(13)	O(12)-Ba(1)-O(11)	66.68(12)
O(19)-Ba(1)-O(13)#2	87.59(14)	O(8)#3-Ba(1)-O(11)	128.58(13)
O(2)#1-Ba(1)-O(12)	77.84(13)	O(2)#1-Ba(1)-O(7)#4	106.47(14)
O(19)-Ba(1)-O(12)	100.75(14)	O(19)-Ba(1)-O(7)#4	65.56(15)
O(19)-Ba(1)-O(11)	140.81(15)	O(13)#2-Ba(1)-O(7)#4	66.49(12)
O(2)#1-Ba(1)-O(8)#3	69.07(13)	O(12)-Ba(1)-O(7)#4	164.80(13)
O(19)-Ba(1)-O(8)#3	68.61(15)	O(8)#3-Ba(1)-O(7)#4	100.99(13)
O(13)#2-Ba(1)-O(8)#3	156.18(12)	O(11)-Ba(1)-O(7)#4	127.98(13)
O(12)-Ba(1)-O(8)#3	66.48(12)	O(2)#1-Ba(1)-O(2W)	65.67(13)
O(2)#1-Ba(1)-O(11)	81.52(13)	O(19)-Ba(1)-O(2W)	132.39(14)
O(13)#2-Ba(1)-O(12)	121.62(11)	O(13)#2-Ba(1)-O(2W)	69.21(12)
O(2)#1-Ba(1)-O(11)#2	138.28(13)	O(12)-Ba(1)-O(2W)	126.86(12)
O(19)-Ba(1)-O(11)#2	72.85(14)	O(8)#3-Ba(1)-O(2W)	126.33(13)
O(13)#2-Ba(1)-O(11)#2	63.65(12)	O(11)-Ba(1)-O(2W)	70.72(13)
O(7)#4-Ba(1)-O(11)#2	114.68(12)	O(7)#4-Ba(1)-O(2W)	67.10(13)
O(8)#3-Ba(1)-O(11)#2	107.99(13)	O(2W)-Ba(1)-O(11)#2	124.83(12)
O(11)-Ba(1)-O(11)#2	68.28(13)	O(12)-Ba(1)-O(11)#2	64.28(11)
O(10)-Ba(2)-O(4)	151.27(13)	O(1)-Ba(2)-O(1W)	66.04(14)
O(10)-Ba(2)-O(1)	99.77(13)	O(16)#5-Ba(2)-O(1W)	145.09(13)
O(4)-Ba(2)-O(1)	67.43(12)	O(2W)-Ba(2)-O(1W)	142.47(14)
O(10)-Ba(2)-O(16)#5	140.18(14)	O(10)-Ba(2)-O(12)#2	104.15(13)
O(4)-Ba(2)-O(16)#5	68.51(12)	O(4)-Ba(2)-O(12)#2	68.90(11)
O(1)-Ba(2)-O(16)#5	98.37(13)	O(1)-Ba(2)-O(12)#2	126.77(12)
O(10)-Ba(2)-O(2W)	68.64(14)	O(16)#5-Ba(2)-O(12)#2	92.58(12)
O(4)-Ba(2)-O(2W)	139.82(12)	O(2W)-Ba(2)-O(12)#2	105.63(12)
O(1)-Ba(2)-O(2W)	127.36(13)	O(1W)-Ba(2)-O(12)#2	75.56(12)
O(16)#5-Ba(2)-O(2W)	72.14(13)	O(10)-Ba(2)-O(13)#2	106.36(13)
O(10)-Ba(2)-O(1W)	74.68(14)	O(4)-Ba(2)-O(13)#2	87.53(11)
O(4)-Ba(2)-O(11)	129.37(12)	O(1)-Ba(2)-O(13)#2	153.64(12)
O(1)-Ba(2)-O(11)	137.67(12)	O(16)#5-Ba(2)-O(13)#2	63.21(12)
O(16)#5-Ba(2)-O(11)	123.64(12)	O(2W)-Ba(2)-O(13)#2	67.48(12)
O(2W)-Ba(2)-O(11)	68.79(12)	O(1W)-Ba(2)-O(13)#2	117.57(12)
O(1W)-Ba(2)-O(11)	79.93(12)	O(12)#2-Ba(2)-O(13)#2	42.85(10)
O(12)#2-Ba(2)-O(11)	65.06(11)	O(10)-Ba(2)-O(11)	45.02(12)
O(13)#2-Ba(2)-O(11)	62.03(11)		

[a]Symmetry transformations used to generate equivalent atoms: For **1**, #1: x, -y+1/2, z+1/2; #2: x, -y+1/2, z-1/2; #3:-x+2, y-1/2, -z-1/2; #4: -x+2, -y, -z; #5: -x+2, y+1/2, -z-1/2. For **2**, #1: -x+3/2, y-1/2, -z-1/2; #2: x+1/2, -y+7/2, z+1/2; #3: x-1/2, -y+7/2, z+1/2; #4: -x+1/2, y-1/2, -z-1/2; #5: -x+1/2, y+1/2, -z-1/2; #6: x-1/2, -y+7/2, z-1/2; #7: -x+3/2, y+1/2, -z-1/2; #8: x+1/2, -y+7/2, z-1/2. For **3**, #1: -x+2, -y+1, -z+1; #2: -x+1, -y+1, -z+1; #3; -x+2, -y+1, -z+2. For **4**, #1: x+1, y, z; #2: -x+3, -y+2, -z+1 ; #3: -x+2, -y+1, -z; #4: x+1, y, z+1; #5: -x+2, -y+2, -z; #6: x-1, y, z-1; #7: x-1, y, z. For **5**, #1: -x, -y, -z; #2: -x-1, -y, -z; #3: x-1, y-1, z-1; #4: -x, -y, -z+1; #5: x+1, y, z+1; #6: x+1, y+1, z+1; #7: x-1,y,z-1.

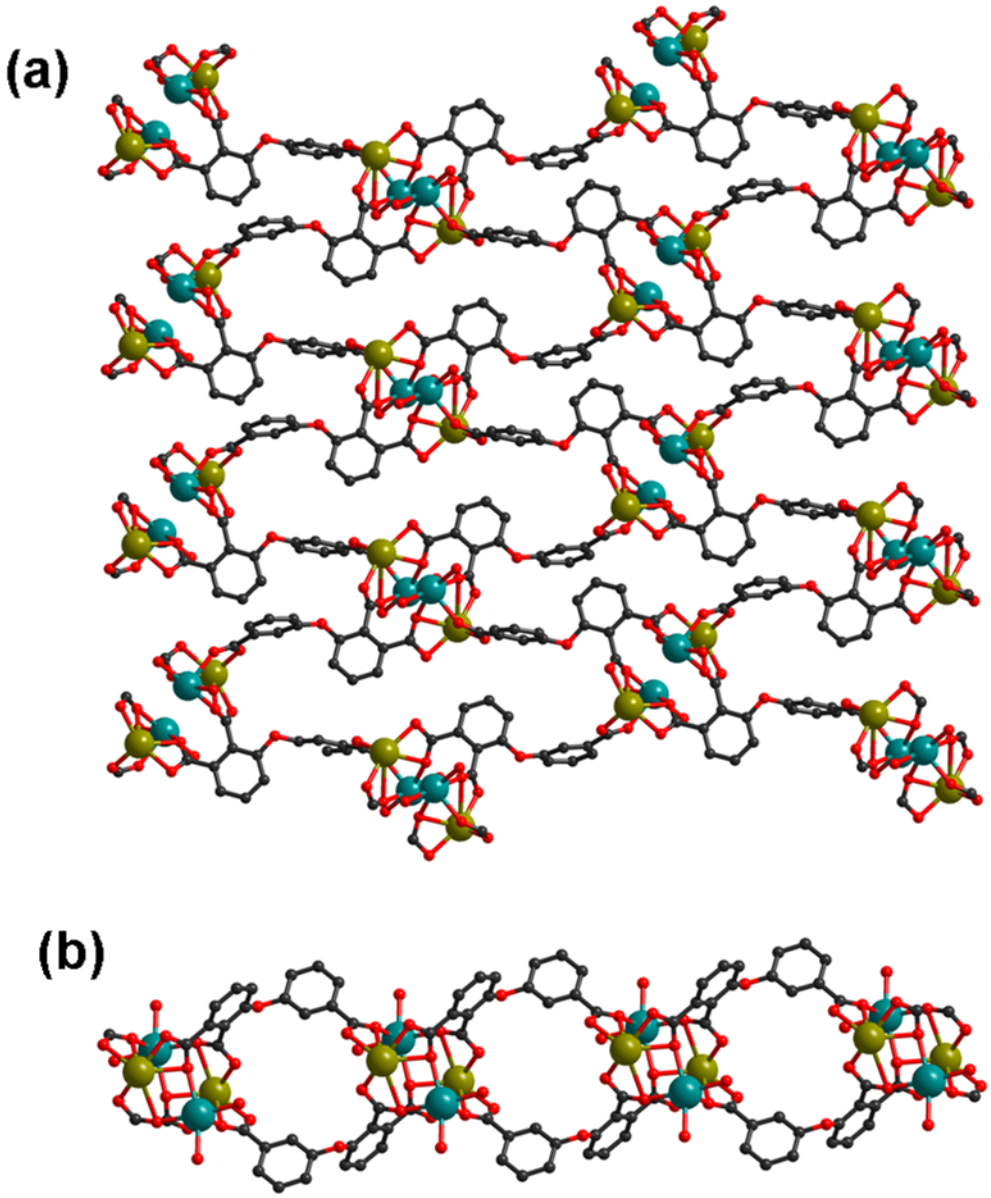

Fig. S1. (a) and (b) Ball-and-stick view of simplified 2D layer structure and 1D linear structure of **2**, after removing one of the two meta-positional carboxylate groups at a time.

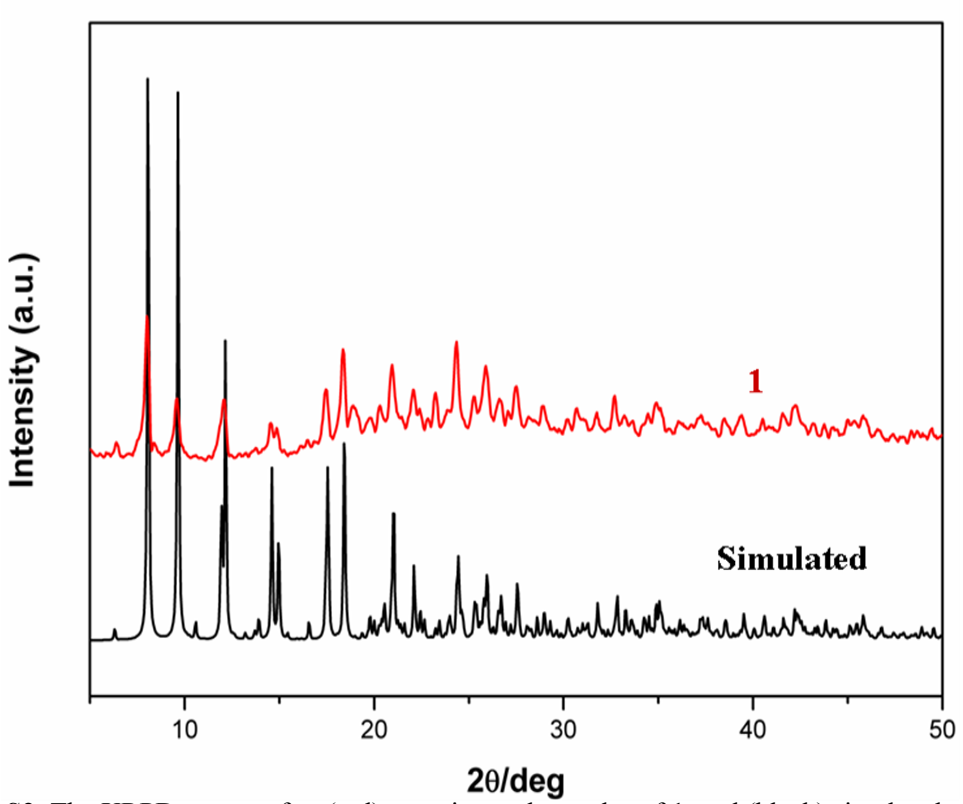

Fig. S2. The XRPD patterns for: (red) experimental samples of **1**, and (black) simulated one based on the single-crystal structure of **1**.

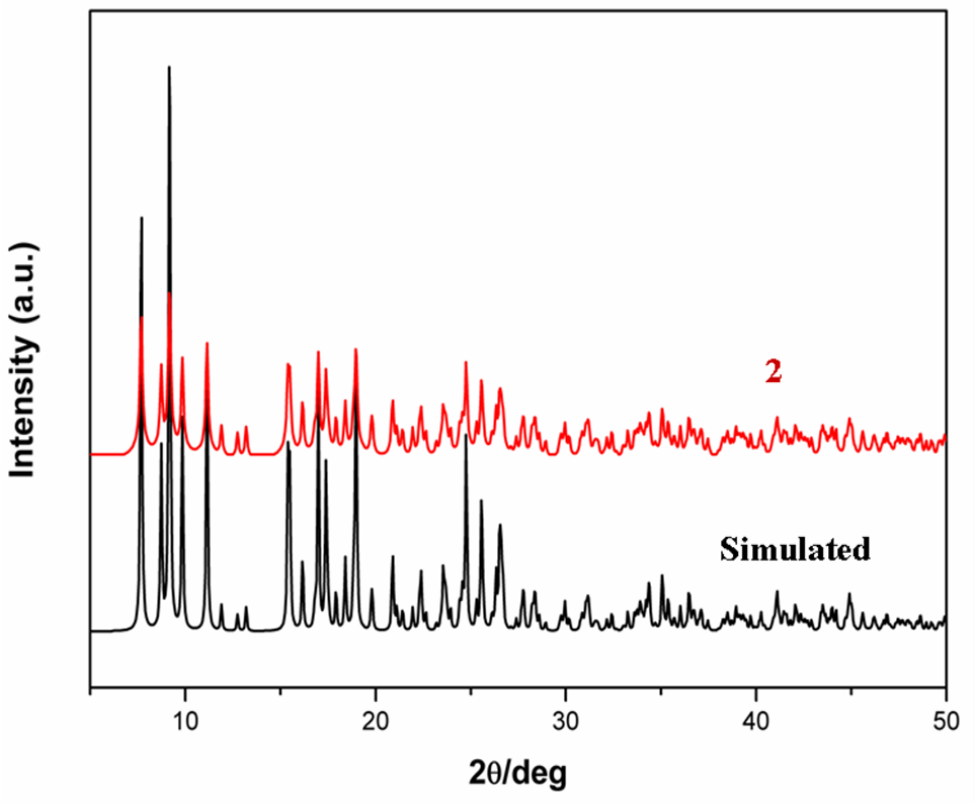

Fig. S3. The XRPD patterns for: (red) experimental samples of **2**, and (black) simulated one based on the single-crystal structure of **2**.

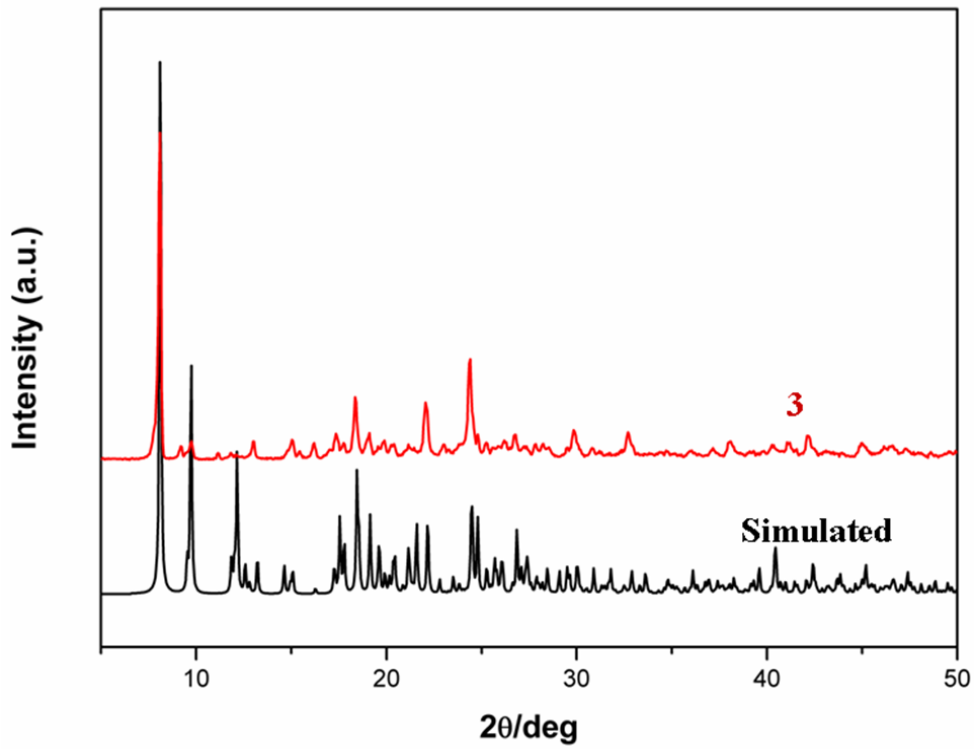

Fig. S4. The XRPD patterns for: (red) experimental samples of **3**, and (black) simulated one based on the single-crystal structure of **3**.

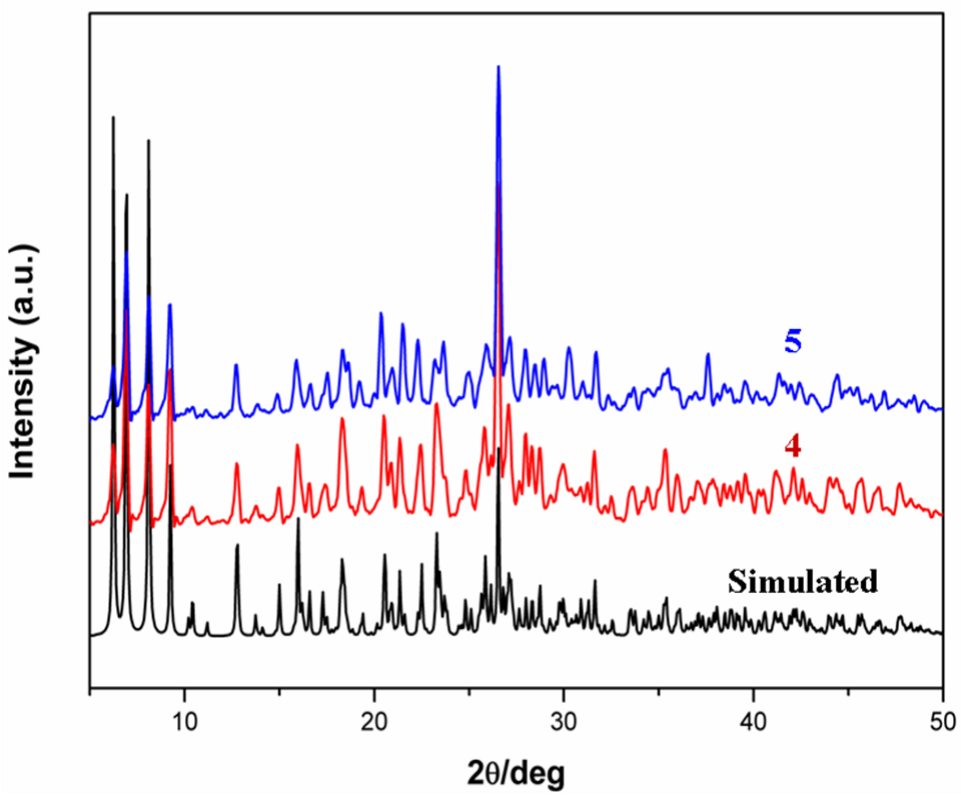

Fig. S5. The XRPD patterns for: (red/blue) experimental samples of **4**/**5**, and (black) simulated one based on the single-crystal structure of **4**.

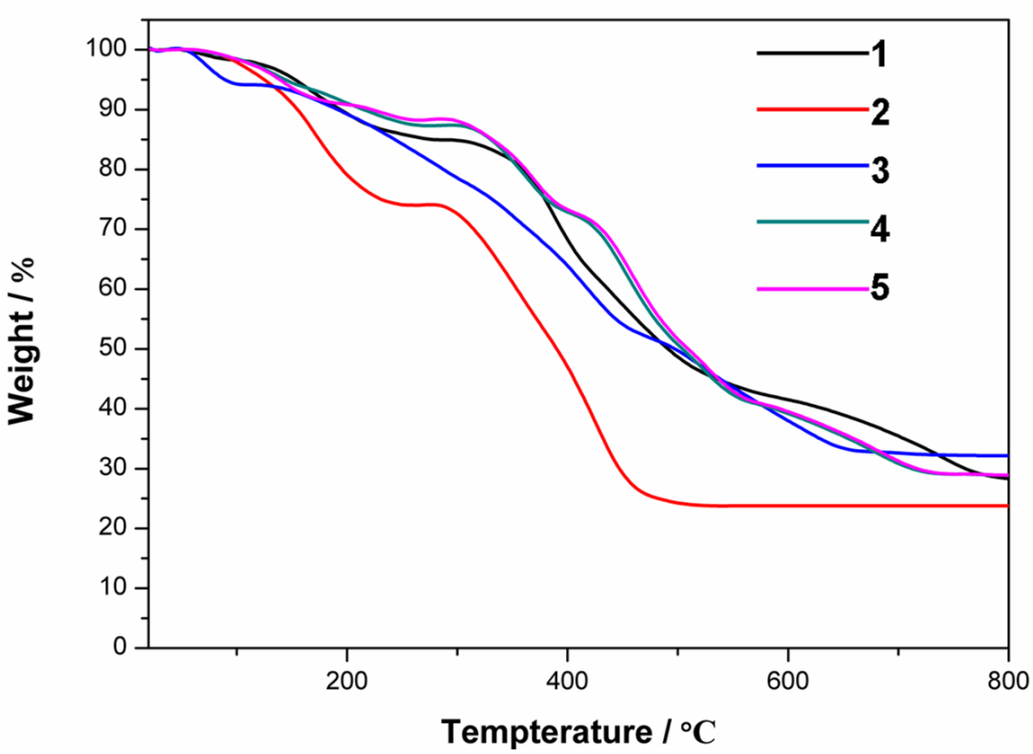

Fig. S6. TGA curves of compounds **1**−**5**.