Supporting information

Using alkaline-earth metal ions to tuned structural variations of 1, 3, 5-benzenetricarboxylate coordination polymers

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Table S1 Selected bond lengths (Å) and angles (º) for **1**.

Cd(1)-O(12)#1	2.260(3)	Cd(1)-O(4)#2	2.261(3)
Cd(1)-O(4W)	2.270(3)	Cd(1)-O(8)	2.311(3)
Cd(1)-O(1)	2.339(3)	Cd(2)-O(10)#3	2.241(3)
Cd(2)-O(2)#4	2.243(3)	Cd(2)-O(11)	2.316(3)
Cd(2)-O(3)#5	2.317(3)	Cd(2)-O(5)	2.361(3)
Cd(2)-O(6)	2.478(3)	Mg(1)-O(9)	2.012(3)
Mg(1)-O(2W)	2.042(3)	Mg(1)-O(1W)	2.066(3)
Mg(1)-O(7)#3	2.108(3)	Mg(1)-O(6)#3	2.111(3)
Mg(1)-O(3W)	2.113(3)	O(12)#1-Cd(1)-O(4)#2	140.83(11)
O(12)#1-Cd(1)-O(4W)	85.74(12)	O(4)#2-Cd(1)-O(4W)	91.43(11)
O(12)#1-Cd(1)-O(8)	82.64(10)	O(4)#2-Cd(1)-O(8)	136.53(10)
O(4W)-Cd(1)-O(8)	91.88(11)	O(12)#1-Cd(1)-O(1)	108.16(11)
O(4)#2-Cd(1)-O(1)	83.22(10)	O(4W)-Cd(1)-O(1)	163.60(11)
O(8)-Cd(1)-O(1)	81.62(10)	O(10)#3-Cd(2)-O(2)#4	135.05(10)
O(10)#3-Cd(2)-O(11)	84.76(10)	O(2)#4-Cd(2)-O(11)	97.55(11)
O(10)#3-Cd(2)-O(3)#5	83.21(10)	O(2)#4-Cd(2)-O(3)#5	84.25(11)
O(11)-Cd(2)-O(3)#5	164.53(10)	O(10)#3-Cd(2)-O(5)	144.44(10)
O(2)#4-Cd(2)-O(5)	80.50(10)	O(11)-Cd(2)-O(5)	92.10(11)
O(3)#5-Cd(2)-O(5)	103.34(11)	O(10)#3-Cd(2)-O(6)	91.49(9)
O(2)#4-Cd(2)-O(6)	132.83(10)	O(11)-Cd(2)-O(6)	93.29(10)
O(3)#5-Cd(2)-O(6)	96.70(10)	O(5)-Cd(2)-O(6)	53.25(9)
O(9)-Mg(1)-O(2W)	173.64(14)	O(9)-Mg(1)-O(1W)	89.80(13)
O(2W)-Mg(1)-O(1W)	85.83(13)	O(9)-Mg(1)-O(7)#3	95.43(12)

O(2W)-Mg(1)-O(7)#3	89.40(12)	O(1W)-Mg(1)-O(7)#3	92.64(12)
O(9)-Mg(1)-O(6)#3	92.17(12)	O(2W)-Mg(1)-O(6)#3	92.05(12)
O(1W)-Mg(1)-O(6)#3	177.32(13)	O(7)#3-Mg(1)-O(6)#3	88.97(13)
O(9)-Mg(1)-O(3W)	87.64(13)	O(2W)-Mg(1)-O(3W)	87.71(13)
O(1W)-Mg(1)-O(3W)	89.70(14)	O(7)#3-Mg(1)-O(3W)	176.14(13)
O(6)#3-Mg(1)-O(3W)	88.57(13)		

Symmetry codes: (#1) *x*, –*y* + 3/2, *z* – 1/2; (#2) –*x* – 1, *y* – 1/2, –*z* – 1/2; (#3) –*x*, –*y* + 1, –*z*; (#4) *x*, –*y* + 3/2, *z* + 1/2; (#5) –*x* – 1, –*y* + 1, –*z*.

Table S2 Selected bond lengths (Å) and angles (º) for **2**.

Cd(1)-O(11)#1	2.162(5)	Cd(1)-O(8)#2	2.226(5)
Cd(1)-O(9)	2.266(5)	Cd(1)-O(1)#3	2.357(5)
Cd(1)-O(10)	2.411(5)	Cd(2)-O(4)	2.211(5)
Cd(2)-O(7)	2.235(5)	Cd(2)-O(1)#4	2.398(5)
Cd(2)-O(5)#3	2.408(5)	Cd(2)-O(6)#3	2.427(5)
Cd(2)-O(2)#4	2.475(6)	Ca(1)-O(3W)	2.319(6)
Ca(1)-O(4W)	2.369(5)	Ca(1)-O(12)	2.384(5)
Ca(1)-O(1W)	2.393(5)	Ca(1)-O(3)#5	2.419(5)
Ca(1)-O(10)#6	2.442(5)	Ca(1)-O(2W)	2.470(6)
O(11)#1-Cd(1)-O(8)#2	101.20(19)	O(11)#1-Cd(1)-O(9)	165.4(2)
O(8)#2-Cd(1)-O(9)	82.1(2)	O(11)#1-Cd(1)-O(1)#3	92.55(19)
O(8)#2-Cd(1)-O(1)#3	88.91(19)	O(9)-Cd(1)-O(1)#3	101.78(18)
O(11)#1-Cd(1)-O(10)	116.27(19)	O(8)#2-Cd(1)-O(10)	136.47(19)
O(9)-Cd(1)-O(10)	56.18(17)	O(1)#3-Cd(1)-O(10)	109.64(16)
O(4)-Cd(2)-O(7)	121.48(19)	O(4)-Cd(2)-O(1)#4	98.35(18)
O(7)-Cd(2)-O(1)#4	128.69(19)	O(4)-Cd(2)-O(5)#3	148.3(2)
O(7)-Cd(2)-O(5)#3	80.71(18)	O(1)#4-Cd(2)-O(5)#3	80.13(18)
O(4)-Cd(2)-O(6)#3	99.84(18)	O(7)-Cd(2)-O(6)#3	92.48(18)
O(1)#4-Cd(2)-O(6)#3	112.55(17)	O(5)#3-Cd(2)-O(6)#3	53.58(18)
O(4)-Cd(2)-O(2)#4	93.76(18)	O(7)-Cd(2)-O(2)#4	89.77(18)
O(1)#4-Cd(2)-O(2)#4	53.99(16)	O(5)#3-Cd(2)-O(2)#4	109.82(18)
O(6)#3-Cd(2)-O(2)#4	162.46(16)	O(3W)-Ca(1)-O(4W)	118.4(2)
O(3W)-Ca(1)-O(12)	161.1(2)	O(4W)-Ca(1)-O(12)	78.6(2)
O(3W)-Ca(1)-O(1W)	86.0(2)	O(4W)-Ca(1)-O(1W)	137.1(2)
O(12)-Ca(1)-O(1W)	75.31(18)	O(3W)-Ca(1)-O(3)#5	78.9(2)
O(4W)-Ca(1)-O(3)#5	69.9(2)	O(12)-Ca(1)-O(3)#5	116.80(18)
O(1W)-Ca(1)-O(3)#5	152.90(19)	O(3W)-Ca(1)-O(10)#6	91.7(2)
O(4W)-Ca(1)-O(10)#6	131.7(2)	O(12)-Ca(1)-O(10)#6	81.16(17)
O(1W)-Ca(1)-O(10)#6	76.78(18)	O(3)#5-Ca(1)-O(10)#6	81.21(17)
O(3W)-Ca(1)-O(2W)	80.9(2)	O(4W)-Ca(1)-O(2W)	75.0(2)
O(12)-Ca(1)-O(2W)	96.91(19)	O(1W)-Ca(1)-O(2W)	75.0(2)
O(3)#5-Ca(1)-O(2W)	123.82(19)	O(10)#6-Ca(1)-O(2W)	151.2(2)

Symmetry codes: (#1) –*x* – 2, –*y*, *z* + 1/2; (#2) –*x*–2, –*y* + 1, *z* + 1/2; (#3) *x*, *y* – 1, *z*; (#4) –*x* – 3/2, *y* – 1/2, *z* – 1/2; (#5) –*x* – 2, –*y* + 1, *z* – 1/2; (#6) –*x*–2, –*y*, *z* – 1/2; (#7) *x*, *y* + 1, *z*; (#8) –*x* – 3/2, *y*

+ 1/2, *z* + 1/2.

Table S3 Selected bond lengths (Å) and angles (º) for **3**.

Cd(1)-O(9)	2.256(9)	Cd(1)-O(12)#1	2.264(9)
Cd(1)-O(8)#2	2.316(9)	Cd(1)-O(3)#3	2.363(8)
Cd(1)-O(4)#2	2.409(8)	Cd(1)-O(7)#2	2.449(10)
Cd(1)-O(10)	2.507(9)	Cd(2)-O(6)#4	2.199(9)
Cd(2)-O(11)	2.224(8)	Cd(2)-O(2)	2.317(9)
Cd(2)-O(4)#5	2.362(9)	Cd(2)-O(1)	2.478(8)
Cd(2)-O(3)#5	2.549(10)	Sr(1)-O(10)	2.457(11)
Sr(1)-O(2W)	2.495(10)	Sr(1)-O(1W)	2.525(10)
Sr(1)-O(5)#2	2.541(9)	Sr(1)-O(5W)	2.57(3)
Sr(1)-O(7)#2	2.584(9)	Sr(1)-O(4W)	2.66(2)
Sr(1)-O(3W)	2.689(10)	O(9)-Cd(1)-O(12)#1	99.3(3)
O(9)-Cd(1)-O(8)#2	178.0(3)	O(12)#1-Cd(1)-O(8)#2	81.2(3)
O(9)-Cd(1)-O(3)#3	92.5(3)	O(12)#1-Cd(1)-O(3)#3	91.1(4)
O(8)#2-Cd(1)-O(3)#3	89.4(3)	O(9)-Cd(1)-O(4)#2	83.3(3)
O(12)#1-Cd(1)-O(4)#2	90.3(3)	O(8)#2-Cd(1)-O(4)#2	94.8(3)
O(3)#3-Cd(1)-O(4)#2	175.7(3)	O(9)-Cd(1)-O(7)#2	124.1(3)
O(12)#1-Cd(1)-O(7)#2	136.6(3)	O(8)#2-Cd(1)-O(7)#2	55.4(3)
O(3)#3-Cd(1)-O(7)#2	89.8(3)	O(4)#2-Cd(1)-O(7)#2	91.9(3)
O(9)-Cd(1)-O(10)	54.2(3)	O(12)#1-Cd(1)-O(10)	152.9(4)
O(8)#2-Cd(1)-O(10)	125.6(4)	O(3)#3-Cd(1)-O(10)	85.3(4)
O(4)#2-Cd(1)-O(10)	91.6(4)	O(7)#2-Cd(1)-O(10)	70.4(3)
O(6)#4-Cd(2)-O(11)	113.6(3)	O(6)#4-Cd(2)-O(2)	101.3(3)
O(11)-Cd(2)-O(2)	93.4(3)	O(6)#4-Cd(2)-O(4)#5	101.5(3)
O(11)-Cd(2)-O(4)#5	122.2(3)	O(2)-Cd(2)-O(4)#5	123.6(3)
O(6)#4-Cd(2)-O(1)	151.0(3)	O(11)-Cd(2)-O(1)	86.3(3)
O(2)-Cd(2)-O(1)	54.7(3)	O(4)#5-Cd(2)-O(1)	83.2(3)
O(6)#4-Cd(2)-O(3)#5	92.7(3)	O(11)-Cd(2)-O(3)#5	80.7(3)
O(2)-Cd(2)-O(3)#5	165.9(3)	O(4)#5-Cd(2)-O(3)#5	52.2(3)
O(1)-Cd(2)-O(3)#5	111.9(3)	O(10)-Sr(1)-O(2W)	131.7(4)
O(10)-Sr(1)-O(1W)	126.8(3)	O(2W)-Sr(1)-O(1W)	84.9(3)
O(10)-Sr(1)-O(5)#2	143.1(3)	O(2W)-Sr(1)-O(5)#2	76.6(3)
O(1W)-Sr(1)-O(5)#2	70.0(3)	O(10)-Sr(1)-O(5W)	67.7(9)
O(2W)-Sr(1)-O(5W)	66.0(9)	O(1W)-Sr(1)-O(5W)	114.1(9)
O(5)#2-Sr(1)-O(5W)	141.3(9)	O(10)-Sr(1)-O(7)#2	69.0(3)
O(2W)-Sr(1)-O(7)#2	93.3(3)	O(1W)-Sr(1)-O(7)#2	158.9(3)
O(5)#2-Sr(1)-O(7)#2	89.1(3)	O(5W)-Sr(1)-O(7)#2	83.9(9)
O(10)-Sr(1)-O(4W)	86.9(5)	O(2W)-Sr(1)-O(4W)	74.1(5)
O(1W)-Sr(1)-O(4W)	65.4(6)	O(5)#2-Sr(1)-O(4W)	128.0(5)
O(5W)-Sr(1)-O(4W)	50.6(9)	O(7)#2-Sr(1)-O(4W)	134.2(6)
O(10)-Sr(1)-O(3W)	71.0(4)	O(2W)-Sr(1)-O(3W)	156.4(3)
O(1W)-Sr(1)-O(3W)	73.9(3)	O(5)#2-Sr(1)-O(3W)	86.4(3)

O(5W)-Sr(1)-O(3W)	132.3(9)	O(7)#2-Sr(1)-O(3W)	102.8(3)
O(4W)-Sr(1)-O(3W)	105.2(5)		

Symmetry codes: (#1) *x*, *y* – 1, *z*; (#2) –*x* + 1, –*y* + 1, *z* – 1/2; (#3) –*x* + 1/2, *y* – 1/2, *z*–1/2; (#4) *x*, *y* + 1, *z*; (#5) –*x* + 1/2, *y* + 1/2, *z*–1/2.

Table S4 Selected bond lengths (Å) and angles (º) for **4**.

Cd(1)-O(2)	2.226(10)	Cd(1)-O(3)#1	2.327(10)
Cd(1)-O(6)#2	2.338(12)	Cd(1)-O(5)#2	2.377(11)
Cd(1)-O(4)#3	2.385(11)	Cd(1)-O(3)#3	2.389(10)
Ba(1)-O(1)#1	2.691(11)	Ba(1)-O(1)	2.691(11)
Ba(1)-O(1)#4	2.691(11)	Ba(1)-O(1W)#4	2.873(13)
Ba(1)-O(1W)	2.873(13)	Ba(1)-O(1W)#1	2.873(13)
Ba(2)-O(3W)	1.98(3)	Ba(2)-O(3W)#9	2.23(4)
Ba(2)-O(3W)#8	2.84(3)	Ba(2)-O(6)	2.931(15)
Ba(2)-O(3W)#7	2.96(2)	Ba(2)-O(3W)#6	3.03(3)
Ba(2)-O(3W)#10	3.14(3)	O(2)-Cd(1)-O(3)#1	81.2(4)
O(2)-Cd(1)-O(6)#2	172.6(4)	O(3)#1-Cd(1)-O(6)#2	91.4(3)
O(2)-Cd(1)-O(5)#2	126.4(4)	O(3)#1-Cd(1)-O(5)#2	104.9(4)
O(6)#2-Cd(1)-O(5)#2	55.7(4)	O(2)-Cd(1)-O(4)#3	97.7(4)
O(3)#1-Cd(1)-O(4)#3	85.3(4)	O(6)#2-Cd(1)-O(4)#3	81.5(4)
O(5)#2-Cd(1)-O(4)#3	135.6(4)	O(2)-Cd(1)-O(3)#3	90.0(3)
O(3)#1-Cd(1)-O(3)#3	136.2(3)	O(6)#2-Cd(1)-O(3)#3	95.4(4)
O(5)#2-Cd(1)-O(3)#3	114.5(3)	O(4)#3-Cd(1)-O(3)#3	53.3(4)
O(1)#1-Ba(1)-O(1)	104.1(3)	O(1)#1-Ba(1)-O(1)#4	104.1(3)
O(1)-Ba(1)-O(1)#4	104.1(3)	O(1)#1-Ba(1)-O(1W)#4	117.6(3)
O(1)-Ba(1)-O(1W)#4	76.2(3)	O(1)#4-Ba(1)-O(1W)#4	137.0(3)
O(1)#1-Ba(1)-O(1W)	76.2(3)	O(1)-Ba(1)-O(1W)	137.0(3)
O(1)#4-Ba(1)-O(1W)	117.6(3)	O(1W)#4-Ba(1)-O(1W)	66.7(4)
O(1)#1-Ba(1)-O(1W)#1	137.0(3)	O(1)-Ba(1)-O(1W)#1	117.6(3)
O(1)#4-Ba(1)-O(1W)#1	76.2(3)	O(1W)#4-Ba(1)-O(1W)#1	66.7(4)
O(1W)-Ba(1)-O(1W)#1	66.7(4)	O(3W)-Ba(2)-O(3W)#9	129.8(9)
O(3W)-Ba(2)-O(3W)#8	75.4(12)	O(3W)#9-Ba(2)-O(3W)#8	146.5(9)
O(3W)-Ba(2)-O(3W)#7	72.4(11)	O(3W)#9-Ba(2)-O(3W)#7	138.8(8)
O(3W)#8-Ba(2)-O(3W)#7	62.7(7)	O(3W)-Ba(2)-O(3W)#6	152.7(10)
O(3W)#9-Ba(2)-O(3W)#6	68.3(9)	O(3W)#8-Ba(2)-O(3W)#6	80.9(4)
O(3W)#7-Ba(2)-O(3W)#6	108.4(6)	O(3W)-Ba(2)-O(3W)#10	142.7(8)
O(3W)#9-Ba(2)-O(3W)#10	66.1(8)	O(3W)#8-Ba(2)-O(3W)#10	109.0(6)
O(3W)#7-Ba(2)-O(3W)#10	77.2(4)	O(3W)#6-Ba(2)-O(3W)#10	58.7(6)

Symmetry codes: (#1) –*x* + *y*, –*x* + 2, *z*; (#2) *y* – 1, *x*, *z* + 1/2; (#3) *x* – *y* + 2, –*y* + 3, *z* + 1/2; (#4) –*y* + 2, *x* – *y* + 2, *z*; (#5) *x* – *y* + 1, –*y* + 3, *z* + 1/2; (#6) –*x* + 2, –*x* + *y* + 1, *z* + 1/2; (#7) –*y* + 3, *x* – *y* + 3, z; (#8) –*x* + *y*, –*x* + 3, *z*; (#9) *x* – *y* + 2, –*y* + 4, *z* + 1/2; (#10) *y* – 1, *x* + 1, *z* + 1/2.

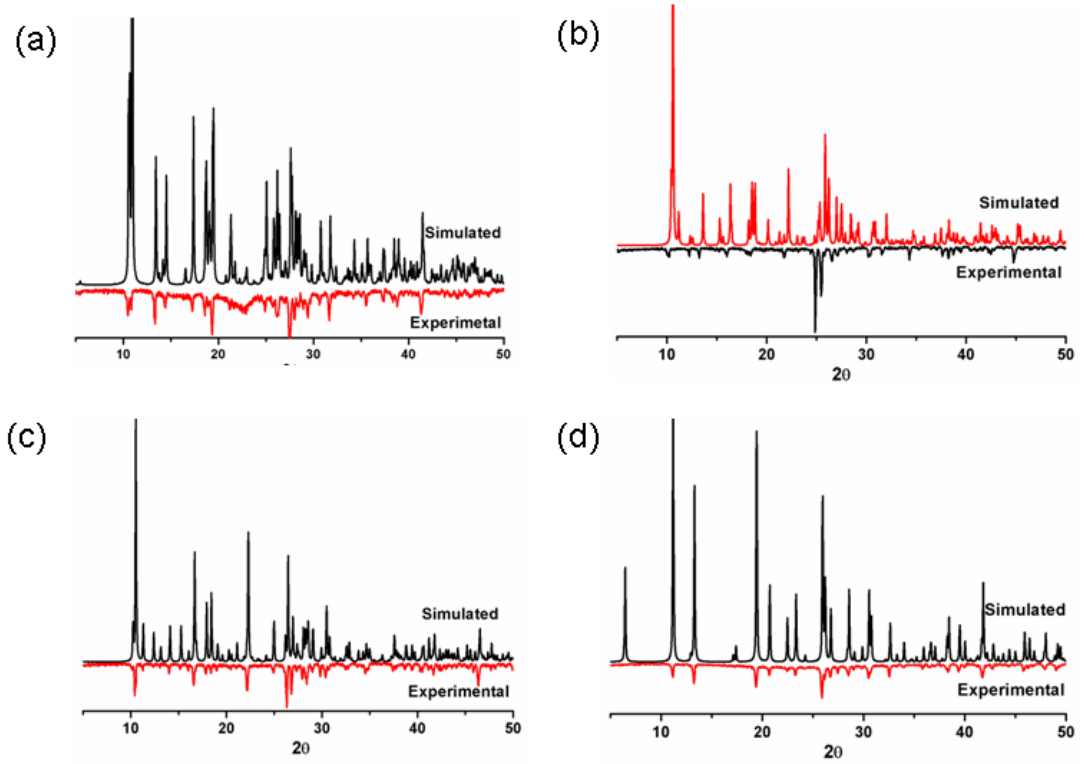

Fig. S1. The simulated and experimental XRD patterns of each compound (a) for **1**, (b) for **2**, and (c) for **3**, (d) for **4**.