Supproting information for

Alkaline-earth Metal Ions Doped Zn(II)-terephthalates†

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

Zn(1)-O(5)	1.941(2)	Zn(1)-O(3)[a]	1.941(3)
Zn(1)-O(1)	1.956(3)	Zn(1)-O(7)	1.965(3)
Mg(1)-O(6)[b]	2.039(2)	Mg(1)-O(6)	2.039(2)
Mg(1)-O(4)[c]	2.047(2)	Mg(1)-O(4)[a]	2.047(2)
Mg(1)-O(2)	2.063(2)	Mg(1)-O(2)[b]	2.063(2)
O(5)-Zn(1)-O(3)[a]	121.70(12)	O(5)-Zn(1)-O(1)	121.15(12)
O(3)[a]-Zn(1)-O(1)	106.38(13)	O(5)-Zn(1)-O(7)	93.06(11)
O(3)[a]-Zn(1)-O(7)	107.51(12)	O(1)-Zn(1)-O(7)	103.44(12)
O(6)[b]-Mg(1)-O(6)	180.0	O(6)[b]-Mg(1)-O(4)[c]	91.57(10)
O(6)-Mg(1)-O(4)[c]	88.43(10)	O(6)[b]-Mg(1)-O(4)[a]	88.43(10)
O(6)-Mg(1)-O(4)[a]	91.57(10)	O(4)[c]-Mg(1)-O(4)[a]	180.000(1)
O(6)[b]-Mg(1)-O(2)	90.15(10)	O(6)-Mg(1)-O(2)	89.85(10)
O(4)[c]-Mg(1)-O(2)	89.68(11)	O(4)[a]-Mg(1)-O(2)	90.32(11)
O(6)[b]-Mg(1)-O(2)[b]	89.85(10)	O(6)-Mg(1)-O(2)[b]	90.15(10)
O(4)[c]-Mg(1)-O(2)[b]	90.32(11)	O(4)[a]-Mg(1)-O(2)[b]	89.68(11)
O(2)-Mg(1)-O(2)[b]	180.0(2)		

Symmetry codes: (a) x, $-y + 2$, $z - 1/2$; (b) $-x - 1/2$, $-y + 5/2$, $-z - 2$; (c) $-x - 1/2$, $y + 1/2$, $-z - 3/2$.

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

Zn(1)-O(5)	1.926(3)	Zn(1)-O(1)	1.945(3)
Zn(1)-O(3)[a]	1.951(3)	Zn(1)-O(7)[b]	1.951(3)
Ca(1)-O(9)	2.274(4)	Ca(1)-O(8)[b]	2.303(3)
Ca(1)-O(10)	2.320(4)	Ca(1)-O(2)	2.331(3)
Ca(1)-O(6)	2.356(3)	Ca(1)-O(4)[c]	2.356(3)
O(5)-Zn(1)-O(1)	112.81(14)	O(5)-Zn(1)-O(3)[a]	101.46(14)
O(1)-Zn(1)-O(3)[a]	114.28(13)	O(5)-Zn(1)-O(7)[b]	125.35(13)
O(1)-Zn(1)-O(7)[b]	106.39(13)	O(3)[a]-Zn(1)-O(7)[b]	95.22(12)
O(9)-Ca(1)-O(8)[b]	90.30(14)	O(9)-Ca(1)-O(10)	94.78(16)
O(8)[b]-Ca(1)-O(10)	170.68(13)	O(9)-Ca(1)-O(2)	159.31(13)
O(8)[b]-Ca(1)-O(2)	80.70(11)	O(10)-Ca(1)-O(2)	96.88(14)
O(9)-Ca(1)-O(6)	81.37(14)	O(8)[b]-Ca(1)-O(6)	98.12(11)
O(10)-Ca(1)-O(6)	90.37(13)	O(2)-Ca(1)-O(6)	81.52(12)
O(9)-Ca(1)-O(4)[c]	94.37(13)	O(8)[b]-Ca(1)-O(4)[c]	85.50(10)
O(10)-Ca(1)-O(4)[c]	86.32(12)	O(2)-Ca(1)-O(4)[c]	103.37(11)
O(6)-Ca(1)-O(4)[c]	174.39(11)		

Symmetry codes: (a) $-x + 1/2$, $y + 1/2$, $-z - 5/2$; (b) $x + 1$, y, z; (c) $-x + 1$, $-y + 1$, $-z - 2$.

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

Sr(1)-O(10)	2.423(4)	Sr(1)-O(6)	2.441(3)
Sr(1)-O(9)	2.471(4)	Sr(1)-O(1)^{a}	2.481(3)
Sr(1)-O(8)^{b}	2.483(3)	Sr(1)-O(4)^{c}	2.485(3)
Zn(1)-O(7)^{b}	1.932(3)	Zn(1)-O(3)^{c}	1.943(3)
Zn(1)-O(2)	1.950(3)	Zn(1)-O(5)	1.953(3)
O(10)-Sr(1)-O(6)	88.45(14)	O(10)-Sr(1)-O(9)	97.39(16)
O(6)-Sr(1)-O(9)	171.98(11)	O(10)-Sr(1)-O(1)^{a}	98.45(13)
O(6)-Sr(1)-O(1)^{a}	87.43(10)	O(9)-Sr(1)-O(1)^{a}	86.28(12)
O(10)-Sr(1)-O(8)^{b}	81.48(15)	O(6)-Sr(1)-O(8)^{b}	95.31(11)
O(9)-Sr(1)-O(8)^{b}	91.01(13)	O(1)^{a}-Sr(1)-O(8)^{b}	177.26(11)
O(10)-Sr(1)-O(4)^{c}	154.92(14)	O(6)-Sr(1)-O(4)^{c}	77.69(11)
O(9)-Sr(1)-O(4)^{c}	98.73(13)	O(1)^{a}-Sr(1)-O(4)^{c}	101.65(10)
O(8)^{b}-Sr(1)-O(4)^{c}	79.15(12)	O(7)^{b}-Zn(1)-O(3)^{c}	110.07(13)
O(7)^{b}-Zn(1)-O(2)	100.69(14)	O(3)^{c}-Zn(1)-O(2)	115.62(13)
O(7)^{b}-Zn(1)-O(5)	128.08(14)	O(3)^{c}-Zn(1)-O(5)	107.25(13)

Symmetry codes: (a) $x - 1/2, -y + 3/2, z - 1/2$; (b) $x + 1, y, z$; (c) $-x + 5/2, y - 1/2, -z + 3/2$.

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

Zn(1)-O(5)	1.939(3)	Zn(1)-O(4)^{a}	1.957(3)
Zn(1)-O(2)	1.976(2)	Zn(1)-O(1W)	2.010(2)
Ba(1)-O(9)	2.694(5)	Ba(1)-O(1)	2.743(3)
Ba(1)-O(1)^{b}	2.743(3)	Ba(1)-O(6)	2.760(3)
Ba(1)-O(6)^{b}	2.760(3)	Ba(1)-O(3)^{c}	2.764(3)
Ba(1)-O(3)^{d}	2.764(3)	Ba(1)-O(1W)	2.959(2)
Ba(1)-O(1W)^{b}	2.959(2)	O(5)-Zn(1)-O(4)^{a}	97.72(12)
O(5)-Zn(1)-O(2)	108.29(12)	O(4)^{a}-Zn(1)-O(2)	121.92(12)
O(5)-Zn(1)-O(1W)	119.94(12)	O(4)^{a}-Zn(1)-O(1W)	106.48(12)
O(2)-Zn(1)-O(1W)	103.67(11)	O(9)-Ba(1)-O(1)	78.41(6)
O(9)-Ba(1)-O(1)^{b}	78.41(6)	O(1)-Ba(1)-O(1)^{b}	156.82(12)
O(9)-Ba(1)-O(6)	126.96(6)	O(1)-Ba(1)-O(6)	67.51(9)
O(1)^{b}-Ba(1)-O(6)	128.62(8)	O(9)-Ba(1)-O(6)^{b}	126.96(6)
O(1)-Ba(1)-O(6)^{b}	128.62(8)	O(1)^{b}-Ba(1)-O(6)^{b}	67.51(8)
O(6)-Ba(1)-O(6)^{b}	106.09(12)	O(9)-Ba(1)-O(3)^{c}	77.16(6)
O(1)-Ba(1)-O(3)^{c}	72.63(9)	O(1)^{b}-Ba(1)-O(3)^{c}	102.08(9)
O(6)-Ba(1)-O(3)^{c}	125.15(8)	O(6)^{b}-Ba(1)-O(3)^{c}	72.03(9)
O(9)-Ba(1)-O(3)^{d}	77.16(6)	O(1)-Ba(1)-O(3)^{d}	102.08(9)
O(1)^{b}-Ba(1)-O(3)^{d}	72.63(9)	O(6)-Ba(1)-O(3)^{d}	72.03(9)
O(6)^{b}-Ba(1)-O(3)^{d}	125.15(8)	O(3)^{c}-Ba(1)-O(3)^{d}	154.32(11)
O(9)-Ba(1)-O(1W)	138.88(5)	O(1)-Ba(1)-O(1W)	69.55(7)
O(1)^{b}-Ba(1)-O(1W)	130.70(8)	O(6)-Ba(1)-O(1W)	62.46(8)
O(6)^{b}-Ba(1)-O(1W)	63.68(8)	O(3)^{c}-Ba(1)-O(1W)	69.27(7)

O(3)^{d}-Ba(1)-O(1W)	133.53(8)	O(9)-Ba(1)-O(1W)^{b}	138.88(5)
O(1)-Ba(1)-O(1W)^{b}	130.70(8)	O(1)^{b}-Ba(1)-O(1W)^{b}	69.55(7)
O(6)-Ba(1)-O(1W)^{b}	63.68(8)	O(6)^{b}-Ba(1)-O(1W)$^{\#2}$	62.46(8)
O(3)^{c}-Ba(1)-O(1W)^{b}	133.53(8)	O(3)^{d}-Ba(1)-O(1W)^{b}	69.27(7)
O(1W)-Ba(1)-O(1W)^{b}	82.24(10)		

Symmetry codes: (a) $-x - 1/2, y + 1/2, -z - 3/2$; (b) $-x - 1, y, -z - 5/2$; (c) $x, -y + 1, z - 1/2$; (d) $-x - 1, -y + 1, -z - 2$.

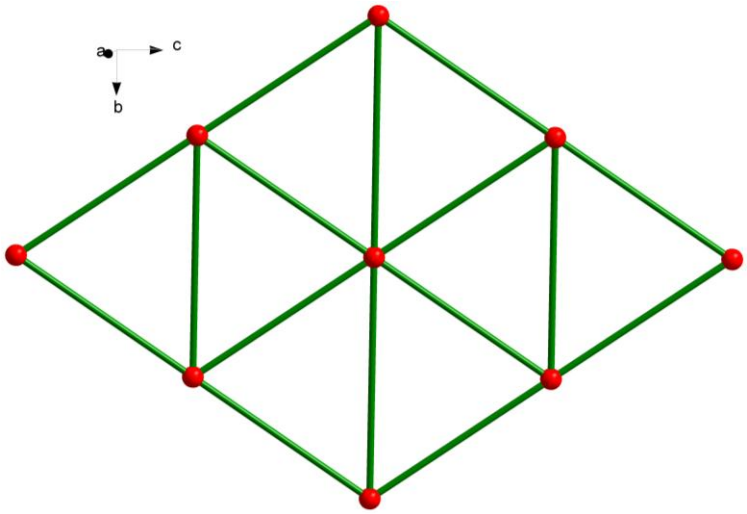

Fig. S1. 6-connected hxl topology for **1**.

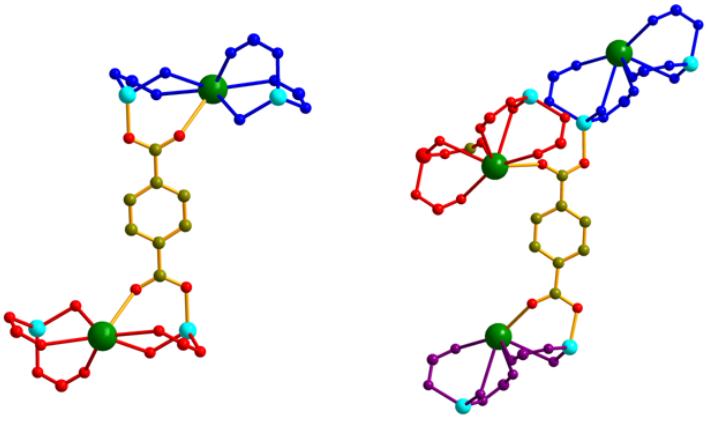

Fig. S2 (a) PBDC ligand linking two different trinuclear $[Zn_2Ba(\mu_2\text{-}COO)_4(\mu_2\text{-}O_{water})_2]$ clusters. (b) PBDC ligand linking three different trinuclear $[Zn_2Ba(\mu_2\text{-}COO)_4(\mu_2\text{-}O_{water})_2]$ clusters.

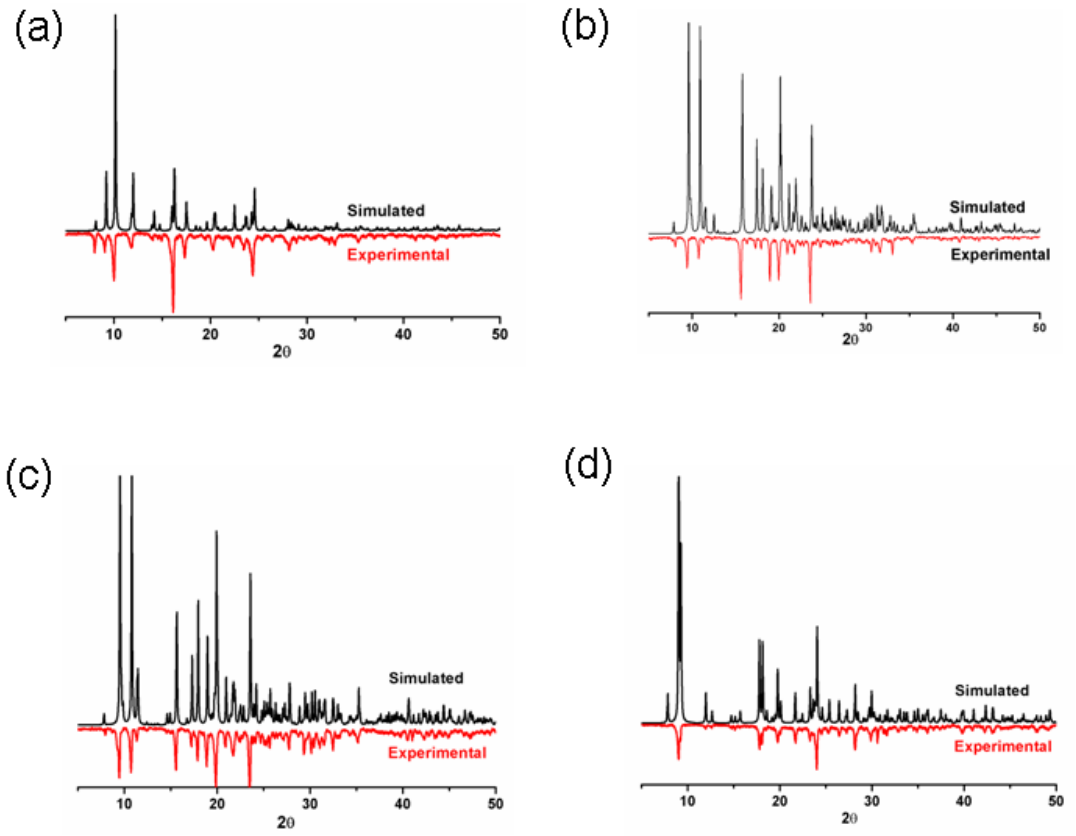

Fig. S3. The simulated and experimental XRD patterns of each compound (a) for **1**, (b) for **2**, and (c) for **3**, (d) for **4**.

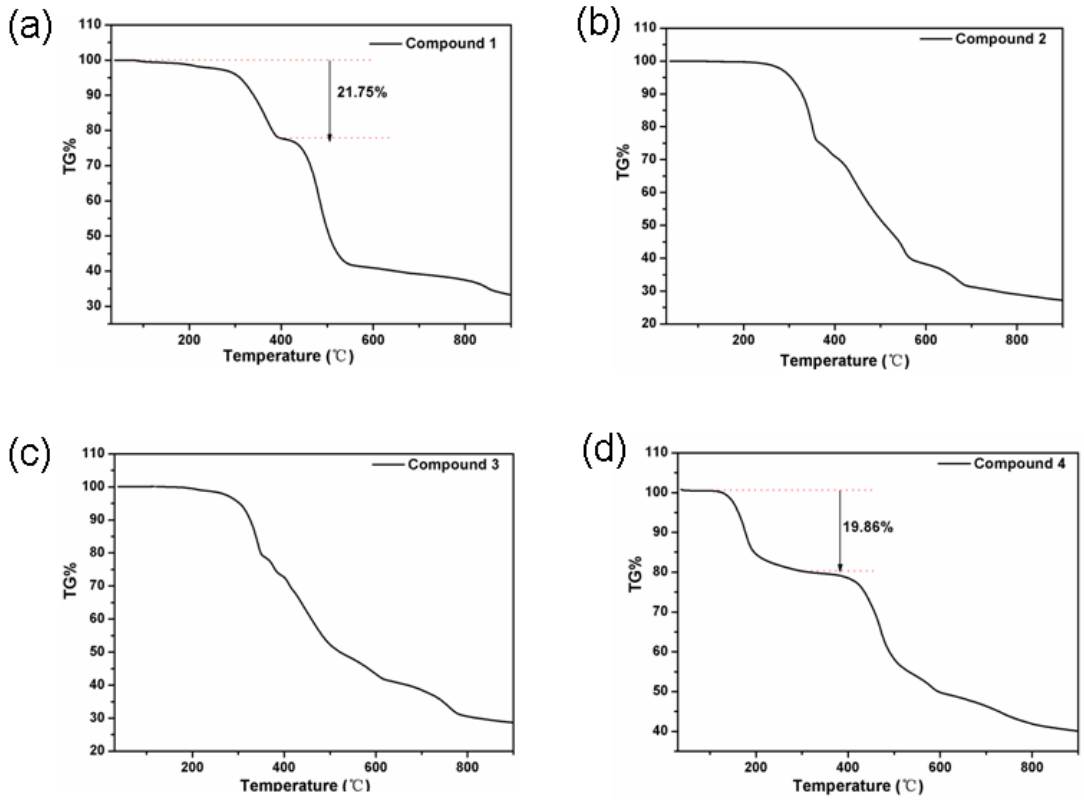

Fig. S4. TG curves of compounds **1**-**5**: (a)-**1**, (b)-**2**, (c)-**3**, (d)-**4**.