Supporting Information

Zinc and Cadmium Metal-Directed Coordination Polymers: In Situ Flexible Tetrazole Ligand Synthesis, Structures, and Properties

Table S1. Selected Bond Distances (Å) and angles (°) for compounds **1**–**3**. Symmetry transformations used to generate equivalent atoms are given as footnotes.

Compound **1a**[a]					
Zn(1)-N(8)	2.033(3)	Zn(1)-N(1)	2.040(3)	Zn(1)-N(4)#1	2.047(3)
Zn(1)-O(2)	2.070(2)	Zn(1)-O(1)	2.071(2)	Zn(2)-O(1)	1.953(2)
Zn(2)-O(2)#2	1.955(2)	Zn(2)-N(5)#3	2.070(3)	Zn(2)-N(7)	2.226(3)
Zn(2)-N(2)#2	2.248(3)	O(2)-Zn(2)#4	1.955(2)	N(2)-Zn(2)#4	2.247(3)
N(4)-Zn(1)#5	2.046(3)	N(5)-Zn(2)#6	2.070(3)	N(8)-Zn(1)-N(1)	133.89(13)
N(8)-Zn(1)-N(4)#1	110.09(13)	N(1)-Zn(1)-N(4)#1	116.01(13)	N(8)-Zn(1)-O(2)	87.57(11)
N(1)-Zn(1)-O(2)	87.76(11)	N(4)#1-Zn(1)-O(2)	96.71(11)	N(8)-Zn(1)-O(1)	88.08(11)
N(1)-Zn(1)-O(1)	85.66(11)	N(4)#1-Zn(1)-O(1)	97.32(11)	O(2)-Zn(1)-O(1)	165.96(10)
O(1)-Zn(2)-O(2)#2	129.48(11)	O(1)-Zn(2)-N(5)#3	115.32(12)	O(2)#2-Zn(2)-N(5)#3	115.18(12)
O(1)-Zn(2)-N(7)	86.12(11)	O(2)#2-Zn(2)-N(7)	96.70(11)	N(5)#3-Zn(2)-N(7)	85.37(12)
O(1)-Zn(2)-N(2)#2	96.50(11)	O(2)#2-Zn(2)-N(2)#2	85.07(11)	N(5)#3-Zn(2)-N(2)#2	89.50(12)
Compound **1b**[b]					
Cd(1)-O(7)	2.258(7)	Cd(1)-O(4)#1	2.269(5)	Cd(1)-O(7)#1	2.272(6)
Cd(1)-N(2)	2.313(7)	Cd(1)-N(3)#1	2.321(7)	Cd(1)-O(3)	2.329(5)
Cd(2)-O(8)	2.208(4)	Cd(2)-O(7)#1	2.274(3)	Cd(2)-O(5)#2	2.331(3)
Cd(2)-O(5)#1	2.340(3)	Cd(2)-N(1)	2.443(10)	Cd(2)-N(4)#3	2.461(10)
N(3)-Cd(1)#4	2.321(7)	N(4)-Cd(2)#5	2.461(10)	O(7)-Cd(2)#4	2.274(3)
O(7)-Cd(1)#4	2.272(6)	O(4)-Cd(1)#4	2.269(5)	O(5)-Cd(2)#6	2.331(3)
O(5)-Cd(2)#4	2.340(3)	O(7)-Cd(1)-O(4)#1	94.82(16)	O(7)-Cd(1)-O(7)#1	176.29(16)
O(7)-Cd(1)-N(2)	95.5(2)	O(4)#1-Cd(1)-N(2	87.8(2)	O(7)#1-Cd(1)-N(2)	83.6(2)
O(7)-Cd(1)-N(3)#1	85.5(2)	N(2)-Cd(1)-N(3)#1	177.4(3)	O(7)-Cd(1)-O(3)	86.44(18)
O(4)#1-Cd(1)-O(3)	177.4(3)	O(7)#1-Cd(1)-O(3)	90.04(17)	N(2)-Cd(1)-O(3)	94.4(2)
N(3)#1-Cd(1)-O(3)	83.2(2)	O(8)-Cd(2)-O(7)#1	94.23(15)	O(8)-Cd(2)-O(5)#2	100.14(15)
O(8)-Cd(2)-O(5)#1	174.1(2)	O(8)-Cd(2)-N(1)	86.4(3)	O(7)#1-Cd(2)-N(1)	86.6(2)
Compound **2a**[c]					
Zn(1)-O(4)	2.100(2)	Zn(1)-O(4)#1	2.100(2)	Zn(1)-N(5)	2.120(3)
Zn(2)-N(1)	2.077(3)	Zn(2)-N(2)	2.012(3)	Zn(2)-O(3)	1.957(2)
Zn(2)-O(2)#4	1.941(2)	Zn(1)-N(4)#3	2.207(3)	Zn(1)-N(4)#2	2.207(3)
Zn(1)-N(5)#1	2.120(3)	O(2)-Zn(2)#5	1.941(2)	N(4)-Zn(1)#2	2.207(3)
O(4)-Zn(1)-O(4)#1	102.43(14)	O(4)-Zn(1)-N(5)	88.40(9)	O(4)#1-Zn(1)-N(5)	84.98(9)
N(2)-Zn(2)-N(1)	102.29(11)	O(3)-Zn(2)-N(1)	103.88(11)	O(2)#4-Zn(2)-N(1)	97.65(11)
O(3)-Zn(2)-N(2)	124.73(10)	O(2)#4-Zn(2)-N(2)	117.17(11)	O(2)#4-Zn(2)-O(3)	106.40(10)

N(4)#2-Zn(1)-N(4)#3	79.11(13)	N(5)#1-Zn(1)-N(4)#3	94.38(9)	N(5)-Zn(1)-N(4)#3	93.77(10)
O(4)#1-Zn(1)-N(4)#3	89.24(10)	O(4)-Zn(1)-N(4)#3	168.28(10)	N(5)#1-Zn(1)-N(4)#2	93.77(10)
N(5)-Zn(1)-N(4)#2	94.38(9)	O(4)#1-Zn(1)-N(4)#2	168.28(10)	O(4)-Zn(1)-N(4)#2	89.24(10)
N(5)-Zn(1)-N(5)#1	169.42(14)	O(4)#1-Zn(1)-N(5)#1	88.40(9)	O(4)-Zn(1)-N(5)#1	84.98(9)

Compound **2b**[d]

N(1)-Cd(2)	2.304(5)	N(3)-Cd(1)#1	2.354(5)	N(4)-Cd(3)#2	2.367(6)
N(5)-Cd(4)	2.454(5)	N(6)-Cd(5)	2.306(5)	N(8)-Cd(2)#3	2.238(5)
N(9)-Cd(4)	2.354(5)	N(10)-Cd(5)	2.348(5)	N(12)-Cd(3)#4	2.284(6)
N(13)-Cd(5)	2.265(6)	N(13)-Cd(4)#5	2.332(6)	O(1)-Cd(1)	2.279(4)
O(1)-Cd(2)	2.578(5)	O(2)-Cd(3)#6	2.352(5)	O(3)-Cd(4)#7	2.250(5)
O(7)-Cd(1)	2.261(4)	O(6)-Cd(5)#4	2.211(5)	O(5)-Cd(4)#8	2.308(4)
O(8)-Cd(4)	2.274(4)	O(8)-Cd(2)	2.223(4)	O(7)-Cd(3)	2.303(4)
O(7W)-Cd(3)	2.355(5)	O(6W)-Cd(3)	2.319(5)	O(8)-Cd(5)	2.297(5)
Cd(5)-O(4)#3	2.379(5)	Cd(5)-O(6)#4	2.211(5)	Cd(4)-N(13)#1	2.332(6)
Cd(4)-O(5)#8	2.308(4)	Cd(4)-O(3)#7	2.250(5)	Cd(3)-N(4)#2	2.367(6)
Cd(3)-O(2)#6	2.352(5)	Cd(3)-N(12)#4	2.284(6)	Cd(2)-O(4)#3	2.445(5)
Cd(2)-N(8)#3	2.238(5)	Cd(1)-N(3)#5	2.354(5)	Cd(1)-N(3)#2	2.354(5)
Cd(1)-O(1)#6	2.279(4)	Cd(1)-O(7)#6	2.261(4)	O(7)-Cd(2)	2.296(4)
O(4)-Cd(2)#3	2.445(5)	O(4)-Cd(5)#3	2.379(5)	O(7)-Cd(1)-O(7)#6	180.0(2)
O(7)-Cd(1)-O(1)	83.89(16)	O(7)#6-Cd(1)-O(1)	96.11(16)	O(1)#6-Cd(1)-O(1)	179.999(1)
O(7)-Cd(1)-N(3)#2	86.75(18)	O(7)#6-Cd(1)-N(3)#2	93.25(18)	O(1)#6-Cd(1)-N(3)#2	83.94(17)
O(1)-Cd(1)-N(3)#2	96.06(17)	O(7)-Cd(1)-N(3)#5	93.25(18)	O(7)#6-Cd(1)-N(3)#5	86.75(18)
O(1)#6-Cd(1)-N(3)#5	96.06(17)	O(1)-Cd(1)-N(3)#5	83.94(17)	N(3)#2-Cd(1)-N(3)#5	180.000(1)
O(8)-Cd(2)-N(8)#3	111.36(18)	O(8)-Cd(2)-O(7)	90.67(16)	N(8)#3-Cd(2)-O(7)	143.06(17)
O(8)-Cd(2)-N(1)	110.65(17)	N(8)#3-Cd(2)-N(1)	98.9(2)	O(7)-Cd(2)-N(1)	100.40(17)
O(8)-Cd(2)-O(4)#3	78.48(16)	N(8)#3-Cd(2)-O(4)#3	76.10(18)	O(7)-Cd(2)-O(4)#3	80.04(16)
N(1)-Cd(2)-O(4)#3	170.80(17)	O(8)-Cd(2)-O(1)	167.36(15)	N(8)#3-Cd(2)-O(1)	80.26(18)
O(7)-Cd(2)-O(1)	76.78(15)	N(1)-Cd(2)-O(1)	70.94(16)	O(4)#3-Cd(2)-O(1)	100.39(15)
N(12)#4-Cd(3)-O(7)	102.98(18)	N(12)#4-Cd(3)-O(6W)	82.1(2)	O(7)-Cd(3)-O(6W)	173.1(2)
N(12)#4-Cd(3)-O(2)#6	93.98(19)	O(7)-Cd(3)-O(2)#6	87.22(16)	O(6W)-Cd(3)-O(2)#6	87.8(2)
N(12)#4-Cd(3)-O(7W)	84.88(19)	O(7)-Cd(3)-O(7W)	90.30(18)	O(6W)-Cd(3)-O(7W)	94.9(2)
O(2)#6-Cd(3)-O(7W)	177.0(2)	N(12)#4-Cd(3)-N(4)#2	157.98(19)	O(7)-Cd(3)-N(4)#2	88.39(17)
O(6W)-Cd(3)-N(4)#2	88.4(2)	O(2)#6-Cd(3)-N(4)#2	105.50(18)	O(7W)-Cd(3)-N(4)#2	76.15(18)
O(3)#7-Cd(4)-O(8)	93.65(17)	O(3)#7-Cd(4)-O(5)#8	101.50(18)	O(8)-Cd(4)-O(5)#8	85.18(15)
O(3)#7-Cd(4)-N(9)	168.04(18)	O(8)-Cd(4)-N(9)	86.95(17)	O(5)#8-Cd(4)-N(9)	90.46(18)
N(13)#1-Cd(4)-N(9)	89.65(19)	O(3)#7-Cd(4)-N(5)	80.46(18)	O(8)-Cd(4)-N(5)	84.31(17)
O(8)-Cd(5)-O(4)#3	78.44(15)	N(13)-Cd(5)-O(4)#3	91.75(19)	O(6)#4-Cd(5)-O(4)#3	91.18(18)
N(6)-Cd(5)-N(10)	86.8(2)	O(8)-Cd(5)-N(10)	87.30(18)	N(13)-Cd(5)-N(10)	102.5(2)
O(6)#4-Cd(5)-N(10)	88.98(19)	O(8)-Cd(5)-N(6)	83.66(18)	N(13)-Cd(5)-N(6)	94.9(2)
O(6)#4-Cd(5)-N(6)	173.31(19)	N(13)-Cd(5)-O(8)	170.02(19)	O(6)#4-Cd(5)-O(8)	91.0(2)
O(6)#4-Cd(5)-N(13)	91.1(2)	N(9)-Cd(4)-N(5)	87.72(18)	N(13)#1-Cd(4)-N(5)	92.24(19)
O(8)-Cd(4)-N(13)#1	175.24(18)	O(5)#8-Cd(4)-N(13)#1	98.18(18)	O(5)#8-Cd(4)-N(5)	169.42(17)

O(3)#7-Cd(4)-N(13)#1	89.0(2)	N(6)-Cd(5)-O(4)#3	91.67(18)	N(10)-Cd(5)-O(4)#3	165.73(18)
Compound **2c**[e]					
O(1)-Zn(1)#1	1.958(3)	Zn(1)-O(1)#2	1.958(3)	Zn(1)-N(1)	2.001(4)
Zn(1)-N(4)#3	2.002(4)	Zn(1)-N(5)	2.048(4)	N(4)-Zn(1)#4	2.002(4)
O(1)#2-Zn(1)-N(1)	121.05(15)	O(1)#2-Zn(1)-N(4)#3	117.72(15)	N(1)-Zn(1)-N(4)#3	105.77(14)
O(1)#2-Zn(1)-N(5)	97.07(15)	N(1)-Zn(1)-N(5)	107.16(15)	N(4)#3-Zn(1)-N(5)	106.30(14)
Compound **3a**[f]					
Cd(1)-N(6)#1	2.291(3)	Cd(1)-N(4)#2	2.316(3)	Cd(1) -N(2) #5	2.331(3)
Cd(1)-N(6)#4	2.291(3)	Cd(1)-N(5)#1	2.433(3)	Cd(1)-N(1)#1	2.504(3)
Cd(1)-N(9)	2.316(3)	Cd(1)-N(2)#3	2.331(3)	Cd(1)-N(4)#6	2.315(3)
Cd(1)-N(5)#4	2.433(3)	Cd(1)-N(1)#4	2.504(3)	N(6)#1-Cd(1)-N(1)#1	71.48(10)
N(6)#1-Cd(1)-N(2)#3	153.51(11)	N(6)#1-Cd(1)-N(9)	88.04(11)	N(4)#2-Cd(1)-N(9)	99.52(11)
N(4)#2-Cd(1)-N(2)#3	100.95(10)	N(9)-Cd(1)-N(2)#3	87.29(10)	N(6)#1-Cd(1)-N(5)#1	86.37(10)
N(4)#2-Cd(1)-N(5)#1	86.23(10)	N(9)-Cd(1)-N(5)#1	172.89(10)	N(2)#3-Cd(1)-N(5)#1	95.77(10)
N(4)#2-Cd(1)-N(1)#1	159.41(10)	N(9)-Cd(1)-N(1)#1	100.72(10)	N(2)#3-Cd(1)-N(1)#1	83.82(10)
Compound **3b**[g]					
Cd(1)-O(1)	2.277(7)	Cd(1)-O(1)#1	2.284(7)	Cd(1)-N(9)#2	2.311(9)
Cd(1)-N(12)#3	2.355(9)	Cd(1)-N(3)#4	2.426(8)	Cd(1)-N(2)	2.493(9)
Cd(2)-O(1)#1	2.298(7)	Cd(2)-N(6)	2.313(9)	Cd(2)-N(1)	2.361(9)
Cd(2)-O(1)#1	2.298(7)	Cd(2)-N(10)	2.363(9)	Cd(2)-N(4)#5	2.407(9)
Cd(2)-N(11)#3	2.542(10)	Cd(1)-N(3)#4	2.426(8)	Cd(2)-N(4)#6	2.407(9)
Cd(1)-N(9)#7	2.311(9)	Cd(2)-N(11)#3	2.542(10)	Cd(1)-N(12)#3	2.355(9)
Cd(1)-O(1)#1	2.284(7)	O(1)-Cd(1)-O(1)#1	84.1(2)	O(1)-Cd(1)-N(9)#2	103.2(3)
O(1)#1-Cd(1)-N(9)#2	172.5(3)	O(1)-Cd(1)-N(12)#3	93.8(3)	O(1)#1-Cd(1)-N(12)#3	85.9(3)
N(3)#4-Cd(1)-N(2)	96.5(3)	N(12)#3-Cd(1)-N(2)	88.5(3)	N(9)#2-Cd(1)-N(2)	93.2(3)
O(1)#1-Cd(1)-N(2)	79.4(3)	O(1)-Cd(1)-N(2)	163.1(3)	N(12)#3-Cd(1)-N(3)#4	175.0(3)
N(9)#2-Cd(1)-N(3)#4	85.2(3)	O(1)#1-Cd(1)-N(3)#4	94.6(3)	O(1)-Cd(1)-N(3)#4	81.3(3)
N(9)#2-Cd(1)-N(12)#3	95.0(3)	N(6)-Cd(2)-N(1)	111.7(3)	O(1)#1-Cd(2)-N(10)	174.3(3)
O(1)#1-Cd(2)-N(1)	81.1(3)	O(1)#1-Cd(2)-N(6)	96.2(3)	N(4)#5-Cd(2)-N(11)#3	78.5(3)
N(10)-Cd(2)-N(11)#3	82.6(3)	N(1)-Cd(2)-N(11)#3	77.5(3)	N(6)-Cd(2)-N(11)#3	168.6(3)
O(1)#1-Cd(2)-N(11)#3	91.9(3)	N(10)-Cd(2)-N(4)#5	97.2(3)	N(1)-Cd(2)-N(4)#5	148.9(3)
N(6)-Cd(2)-N(4)#5	94.9(3)	O(1)#1-Cd(2)-N(4)#5	80.3(3)	N(1)-Cd(2)-N(10)	98.9(3)

[a] #1 x-y,x,-z+1; #2 x,y,z+1; #3 -y+2/3,x-y+1/3,z+1/3; #4 x,y,z-1; #5 y,-x+y,-z+1; #6 -x+y+1/3,-x+2/3,z-1/3. [b] #1 -x+1/2,-y+2,z+1/2; #2 x+1/2,y,z+1/2; #3 x,y,z+1; #4 -x+1/2,-y+2,z-1/2; #5 x,y,z-1; #6 x-1/2,y,z-1/2. [c] #1 -x,y,-z+3/2; #2 -x,-y+1,-z+1; #3 x,-y+1,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,y,-z+1/2; #7 x,y,z+1; #8 x,y,z-1. [d] #1 x+1,y,z; #2 -x+2,-y+1,-z+1 ;#3 -x+1,-y+1,-z ;#4 -x+1,-y,-z; #5 x-1,y,z; #6 -x+1,-y+1,-z+1; #7 -x+2,-y+1,-z; #8 -x+2,-y,-z. [e] #1 x+1/2,-y+1/2,z+1/2; #2 x-1/2,-y+1/2,z-1/2; #3 x,-y+1,z-1/2; #4 x,-y+1,z+1/2. [f] #1 y-1/3,-x+y+1/3,-z+1/3; #2 -y+4/3,x-y+5/3,z+2/3; #3 -x+y-1/3,-x+4/3,z+1/3; #4 x-y+2/3,x+1/3,-z+1/3; #5 -y+4/3,x-y+5/3,z-1/3; #6 -x+y-1/3,-x+4/3,z-2/3. [g] #1 -x+2,-y+1,-z+2; #2 x+1/2,-y+1/2,z+1/2; #3 -x+1,-y+1,-z+2; #4 -x+2,-y,-z+2; #5 x,y+1,z; #6 x,y-1,z; #7 x-1/2,-y+1/2,z-1/2.

Table S2. Hydrogen Bonds of Compounds **1-3**.

D—H…A	d(D—H) (Å)	D(H…A) (Å)	d(D…A) (Å)	∠(D—H…A) (deg)
		Compound **1a**		
C(3)—H(3B)…N(2)	0.97	2.58	3.204(6)	122
		Compound **1b**		
O(2)—H(2)…O(8)	0.82	2.58	2.992(11)	113
O(8)—H(8A)…O(4)	0.85	2.47	3.111(7)	133
O(8)—H(8B)…O(6)	0.85	2.53	2.835(9)	102
C(2)—H(2A)…O(3)	0.97	2.45	3.391(9)	163
C(2)—H(2B)…O(4)	0.97	2.52	3.442(9)	158
		Compound **2a**		
C(5)—H(5)…N(3)	0.93	2.47	3.099(5)	125
		Compound **2b**		
O(8W)—H(8WA)…N(15)	0.84(7)	2.53(8)	3.339(17)	165(15)
O(8W)—H(8WB)…O(2)	0.85(15)	2.24(15)	2.085(13)	172(15)
O(6W)—H(6A)…N(15)	0.82(4)	1.99(4)	2.793(11)	165(12)
O(6W)—H(6B)…O(8W)	0.82(5)	2.00(6)	2.796(14)	164(8)
O(7W)—H(7A)…O(5)	0.82(5)	1.96(6)	2.730(8)	156(7)
O(7W)—H(7B)…N(2)	0.82(8)	2.18(7)	2.948(9)	157(7)
C(2)—H(2B)…O(6W)	0.97	2.56	3.368(10)	141
		Compound **2c**		
O(4W)—H(4A)…O(4W)	0.93	1.85	2.771(10)	167

O(4W)—H(4B)…N(2)	0.97	2.03	2.958(9)	158
C(3)—H(3)…O(1)	0.93	2.49	3.051(6)	119
		Compound **3a**		
C(2)—H(2A)…N(3)	0.97	2.62	3.318(3)	129
		Compound **3b**		
O(1)—H(1)…N(8)	0.83(10)	2.29(9)	3.051(12)	154(10)
C(4)—H(4A)…N(13)	0.97	2.25	3.133(15)	151
C(4)—H(4B)…N(7)	0.97	2.55	3.283(16)	133

Fig. S1 View of the helical chains P, M in compound **1a** generated between three arbitrary adjacent hexagonal channels along the *c*-axis. P and M indicate the right- and left-handed helical channels, respectively. The pink balls stand for Zn1 cations and the blue balls stand for Zn2 cations.

Fig. S2 The themogravimetric analysis (TGA) curves of **1.**

Fig. S3 The themogravimetric analysis (TGA) curves of **2.**

Fig. S4 The themogravimetric analysis (TGA) curves of **3.**

Fig. S5 Powder X-ray diffraction measurements (PXRD) patterns for **1a**.

Fig. S6 Powder X-ray diffraction measurements (PXRD) patterns for **1b**.

Fig. S7 Powder X-ray diffraction measurements (PXRD) patterns for **2a**.

Fig. S8 Powder X-ray diffraction measurements (PXRD) patterns for **2b**.

Fig. S9 Powder X-ray diffraction measurements (PXRD) patterns for **2c**.

Fig. S10 Powder X-ray diffraction measurements (PXRD) patterns for **3a**.

Fig. S11 Powder X-ray diffraction measurements (PXRD) patterns for **3b**.