

[Supporting information]

Syntheses, Structures and Luminescent Properties of Seven Metal-Organic Frameworks Constructed with A Rigid Imidazole Ligand and Versatile Carboxylate Acids

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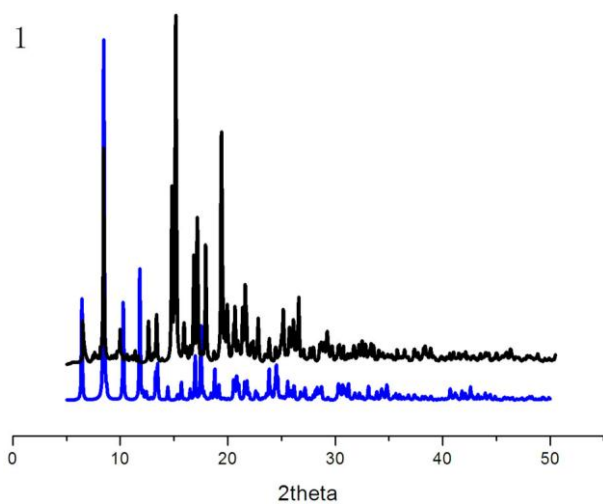


Figure S1. The simulated (blue) and experimental (black) XRPD patterns for **1**.

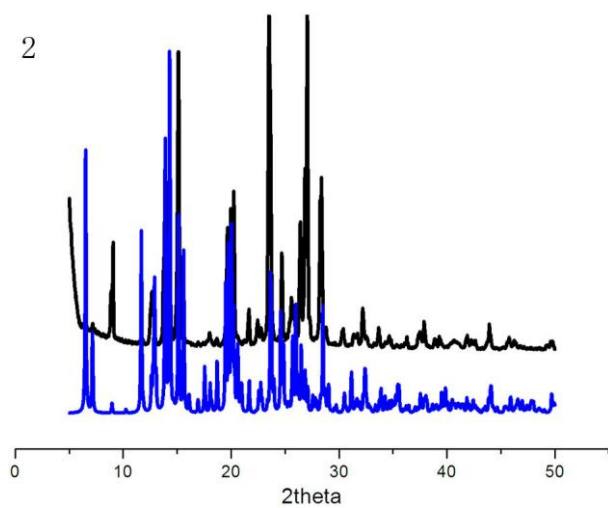


Figure S2. The simulated (blue) and experimental (black) XRPD patterns for **2**.

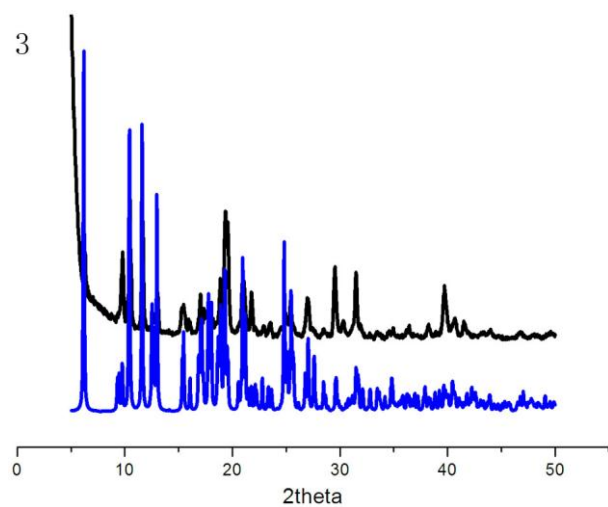


Figure S3. The simulated (blue) and experimental (black) XRPD patterns for **3**.

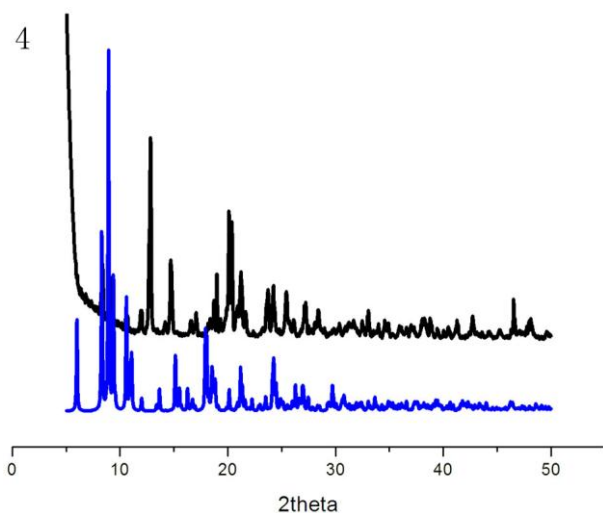


Figure S4. The simulated (blue) and experimental (black) XRPD patterns for **4**.

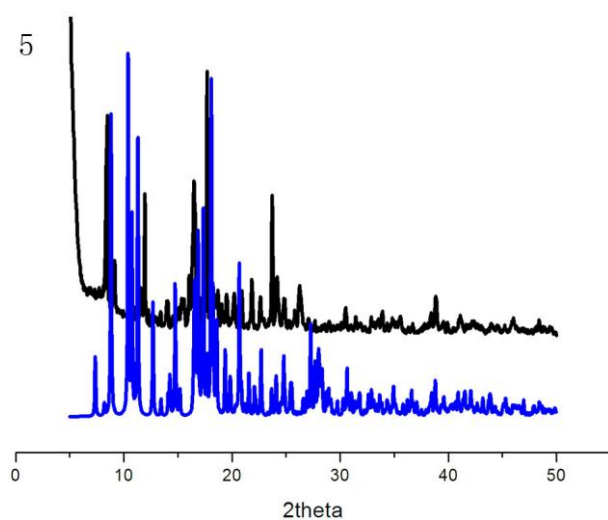


Figure S5. The simulated (blue) and experimental (black) XRPD patterns for **5**.

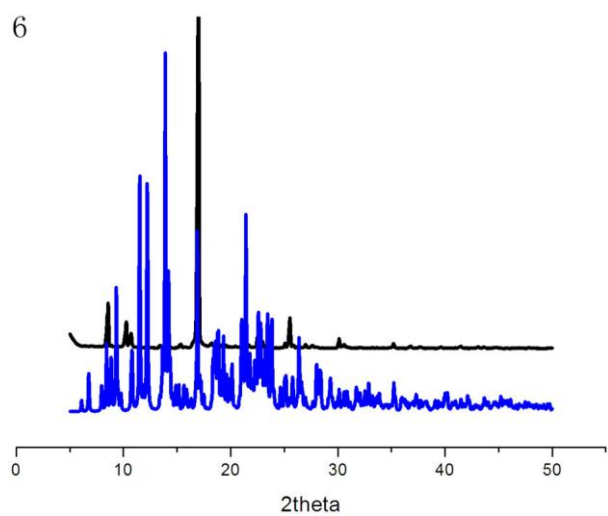


Figure S6. The simulated (blue) and experimental (black) XRPD patterns for **6**.

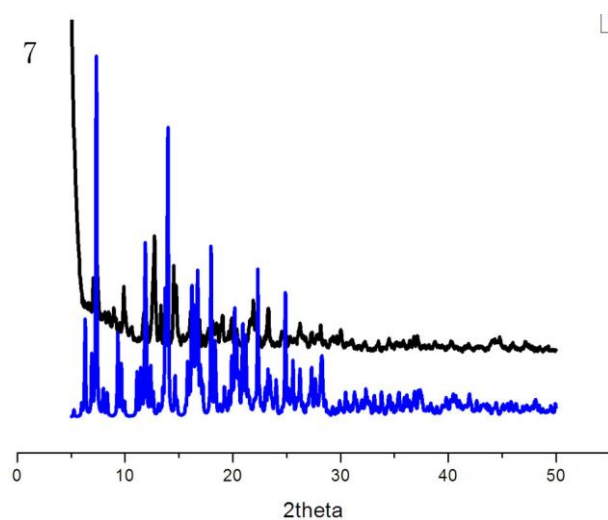


Figure S7. The simulated (blue) and experimental (black) XRPD patterns for **7**.

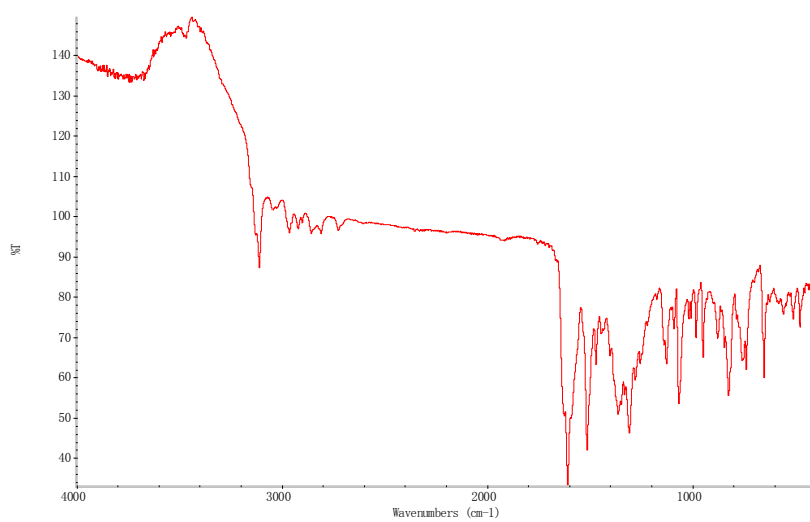


Figure S8. IR (4000-400 cm⁻¹) spectrum of the compound **1**.

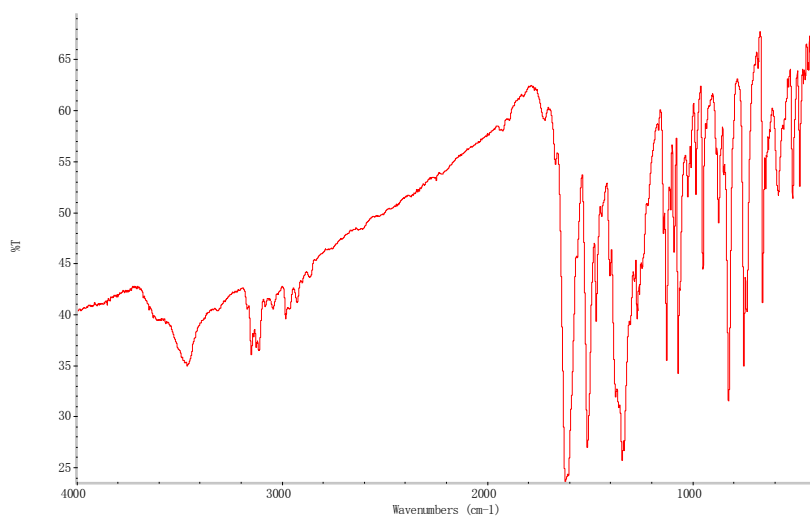


Figure S9. IR (4000-400 cm⁻¹) spectrum of the compound **2**.

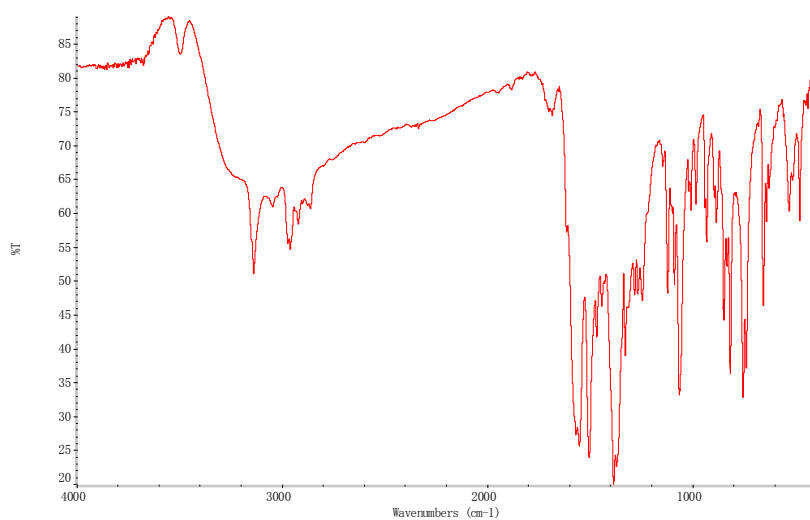


Figure S10. IR (4000-400 cm⁻¹) spectrum of the compound **3**.

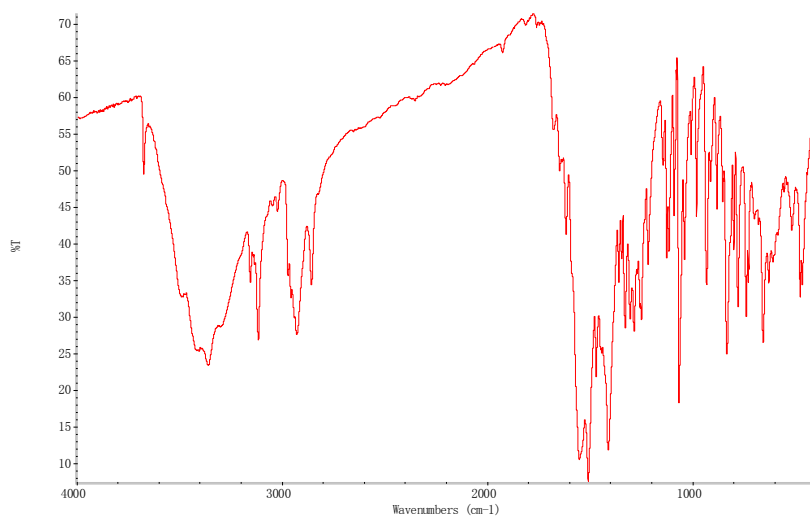


Figure S11. IR (4000-400 cm⁻¹) spectrum of the compound **4**.

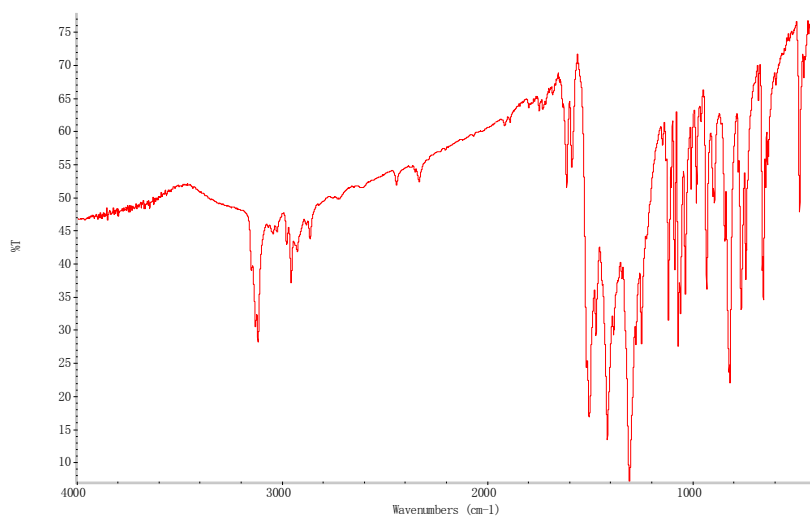


Figure S12. IR (4000-400 cm⁻¹) spectrum of the compound **5**.

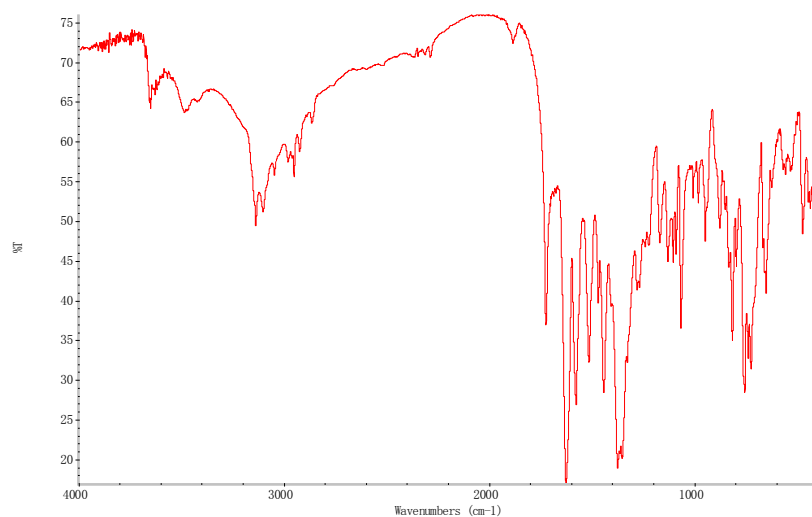


Figure S13. IR (4000-400 cm^{-1}) spectrum of the compound **6**.

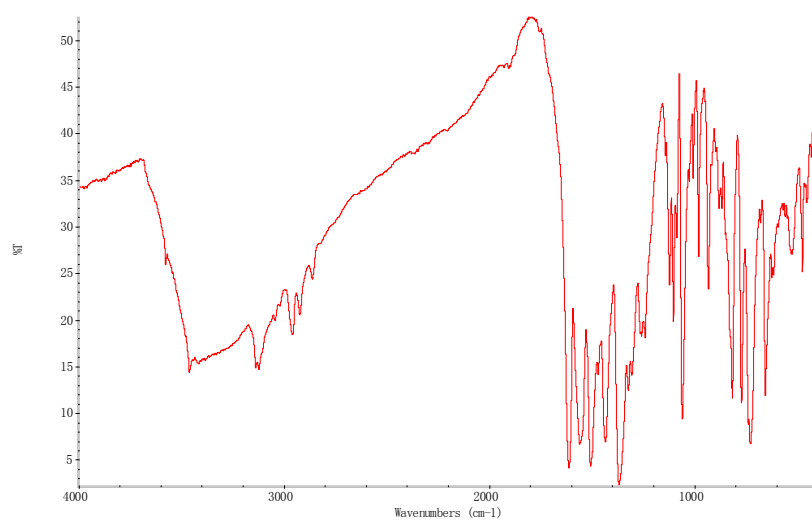


Figure S14. IR (4000-400 cm^{-1}) spectrum of the compound **7**.

Table S1. Selected bond distances (\AA) and angles ($^\circ$) for **1**.

Zn(1)-N(1)	2.025(3)
Zn(1)-O(1)	2.224(3)
Zn(1)-(5)	2.081(3)
Zn(1)-O(7)	1.947(3)
Zn(1)-O(9)	1.999(2)
Zn(2)-O(6)	2.075(2)
Zn(2)-O(8)	2.145(2)
Zn(2)-O(9)	2.081(2)
Zn(3)-O(2)	1.941(3)
Zn(3)#1-O(4)	2.032(3)

Zn(3)-O(9)	1.942(2)
Zn(3)-N(4)#3	1.978(3)
O(7)-Zn(1)-O(9)	119.67(11)
O(7)-Zn(1)-N(1)	117.20(12)
O(9)-Zn(1)-N(1)	122.97(11)
O(7)-Zn(1)-O(5)	92.99(12)
O(9)-Zn(1)-O(5)	90.50(10)
N(1)-Zn(1)-O(5)	90.53(11)
O(7)-Zn(1)-O(1)	87.61(11)
O(9)-Zn(1)-O(1)	93.20(9)
N(1)-Zn(1)-O(1)	85.11(11)
O(5)-Zn(1)-O(1)	175.37(10)
O(6)#2-Zn(2)-O(6)	180.000(1)
O(6)#2-Zn(2)-O(9)	85.43(9)
O(6)-Zn(2)-O(9)	94.57(9)
O(9)-Zn(2)-O(9)#2	180.000(1)
O(6)-Zn(2)-O(8)#2	90.77(10)
O(6)-Zn(2)-O(8)	89.23(10)
O(9)-Zn(2)-O(8)	93.97(10)
O(9)#2-Zn(2)-O(8)	86.03(10)
O(8)#2-Zn(2)-O(8)	180.0
O(2)-Zn(3)-O(9)	116.86(11)
O(2)-Zn(3)-N(4)#3	108.34(12)
O(9)-Zn(3)-N(4)#3	129.20(12)
O(2)-Zn(3)-O(4)#4	99.10(12)
O(9)-Zn(3)-O(4)#4	98.46(10)
N(4)#3-Zn(3)-O(4)#4	96.08(12)

Symmetry transformations used to generate equivalent atoms: #1 $x+1/2, y, -z+5/2$; #2 $-x+2, -y, -z+2$; #3 $x, -y-1/2, z-1/2$; #4 $x-1/2, y, -z+5/2$.

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Zn(1)-N(1)	1.9919(18)
Zn(1)-O(2)	1.9543(16)
Zn(1)-O(4)	1.9557(17)
Zn(1)-N(4)#1	2.0078(19)
O(2)-Zn(1)-O(4)	107.48(7)
O(2)-Zn(1)-N(1)	114.21(7)
O(4)-Zn(1)-N(1)	115.74(8)
O(2)-Zn(1)-N(4)#1	112.12(8)
O(4)-Zn(1)-N(4)#1	94.00(7)
N(1)-Zn(1)-N(4)#1	111.60(8)

Symmetry transformations used to generate equivalent atoms: #1 $x+1/2, y+1/2, z$.

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

Cd(1)-N(1)	2.318(4)
Cd(1)-N(4)	2.253(3)
Cd(1)-O(2)	2.233(3)
Cd(1)-O(1W)	2.393(3)
Cd(1)-O(3)	2.426(3)
Cd(1)-O(4)	2.327(3)
O(2)-Cd(1)-N(4)	114.05(12)
O(2)-Cd(1)-N(1)	83.48(11)
N(4)-Cd(1)-N(1)	96.85(12)
O(2)-Cd(1)-O(4)	100.28(11)
N(4)-Cd(1)-O(4)	145.39(11)
N(1)-Cd(1)-O(4)	90.98(11)
O(2)-Cd(1)-O(1W)	81.34(10)
N(4)-Cd(1)-O(1W)	90.69(12)
N(1)-Cd(1)-O(1W)	164.75(11)
O(4)-Cd(1)-O(1W)	90.28(10)
O(2)-Cd(1)-O(3)	153.00(11)
N(4)-Cd(1)-O(3)	90.33(11)
N(1)-Cd(1)-O(3)	105.92(11)
O(4)-Cd(1)-O(3)	55.17(10)
O(1W)-Cd(1)-O(3)	87.21(10)

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

Cd(1)-N(3)	2.278(4)
Cd(1)-O(4)	2.415(3)
Cd(1)-O(6)	2.381(3)
Cd(1)-O(7)	2.276(3)
Cd(1)-OW1	2.339(3)
Cd(2)-N(1)	2.234(4)
Cd(2)-O(1)	2.311(3)
Cd(2)-O(8)#1	2.288(3)
Cd(2)-O(4)#2	2.318(3)
Cd(2)-O(5)#2	2.362(3)
Cd(2)-OW1#2	2.452(3)

O(7)-Cd(1)-N(3)	90.21(14)
O(7)-Cd(1)-OW1	133.13(11)
N(3)-Cd(1)-OW1	91.22(13)
O(7)-Cd(1)-O(6)	101.70(12)
N(3)-Cd(1)-O(6)	93.66(14)
OW1-Cd(1)-O(6)	124.92(11)
O(7)-Cd(1)-O(4)	110.91(12)
N(3)-Cd(1)-O(4)	158.86(13)
OW1-Cd(1)-O(4)	73.83(11)
O(6)-Cd(1)-O(4)	83.32(12)
N(1)-Cd(2)-O(8)#1	105.44(13)
N(1)-Cd(2)-O(1)	81.62(13)
O(8)#1-Cd(2)-O(1)	92.10(13)
N(1)-Cd(2)-O(4)#2	123.77(12)
O(8)#2-Cd(2)-O(4)#2	89.78(11)
O(1)-Cd(2)-O(4)#2	152.91(12)
N(1)-Cd(2)-O(5)#2	94.63(13)
O(8)#1-Cd(2)-O(5)#2	159.83(12)
O(1)-Cd(2)-O(5)#2	88.80(13)
O(4)#2-Cd(2)-O(5)#2	80.51(12)
N(1)-Cd(2)-OW1#2	158.29(12)
O(8)#1-Cd(2)-OW1#2	86.22(12)
O(1)-Cd(2)-OW1#2	79.66(11)
O(4)#2-Cd(2)-OW1#2	73.50(10)
O(5)#2-Cd(2)-OW1#2	74.12(11)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+1; #2 x+1,y,z.

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Cd(1)-N(1)	2.271(3)
Cd(1)-O(1)	2.3115(19)
Cd(1)-O(2)	2.413(2)
Cd(2)-N(4)	2.264(2)
Cd(2)-O(3)	2.357(3)
Cd(2)-O(4)	2.309(3)
N(1)-Cd(1)-N(1)#1	180.00(11)
N(1)-Cd(1)-O(1)	90.59(8)
N(1)-Cd(1)-O(1)#1	89.41(8)
O(1)-Cd(1)-O(1)#1	180.00(6)
N(1)-Cd(1)-O(2)#1	88.65(9)
O(1)-Cd(1)-O(2)#1	124.71(7)

N(1)-Cd(1)-O(2)	91.35(9)
O(1)-Cd(1)-O(2)	55.29(7)
O(2)#1-Cd(1)-O(2)	180.00(12)
N(4)-Cd(2)-N(4)#2	90.66(13)
N(4)-Cd(2)-O(4)	143.58(9)
N(4)-Cd(2)-O(4)#2	98.94(11)
O(4)-Cd(2)-O(4)#2	93.88(16)
N(4)-Cd(2)-O(3)	89.38(9)
O(4)-Cd(2)-O(3)	54.49(9)
N(4)-Cd(2)-O(3)#2	99.36(11)
O(4)-Cd(2)-O(3)#2	115.69(11)
O(3)-Cd(2)-O(3)#2	167.61(17)

Symmetry transformations used to generate equivalent atoms: #1 $-x+2, -y+1, -z$; #2 $-x, y, -z-1/2$.

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Zn(1)-N(1)	1.984(3)
Zn(1)-O(1)	1.961(3)
Zn(1)-O(10)#2	1.941(3)
Zn(1)-O(2)#1	1.975(3)
Zn(2)-N(5)	2.008(3)
Zn(2)-N(8)#3	2.024(3)
Zn(2)-O(4)	1.956(3)
Zn(2)-O(8)	1.952(3)
O(10)#2-Zn(1)-O(1)	116.78(12)
O(10)#2-Zn(1)-O(2)#1	98.85(11)
O(1)-Zn(1)-O(2)#1	117.15(12)
O(10)#2-Zn(1)-N(1)	116.93(14)
O(1)-Zn(1)-N(1)	98.94(13)
O(2)#1-Zn(1)-N(1)	108.94(14)
O(8)-Zn(2)-O(4)	109.81(12)
O(8)-Zn(2)-N(5)	104.33(12)
O(4)-Zn(2)-N(5)	121.53(13)
O(8)-Zn(2)-N(8)#3	96.73(12)
O(4)-Zn(2)-N(8)#3	112.55(12)
N(5)-Zn(2)-N(8)#3	108.73(13)

Symmetry transformations used to generate equivalent atoms: #1 $-x+1, -y, -z+2$; #2 $-x+2, y+1/2, -z+5/2$; #3 $-x+1, y+1/2, -z+5/2$.

Table S7. Selected bond distances (Å) and angles (°) for **7**.

Cd(1)-N(1)	2.270(3)
Cd(1)-N(12)	2.270(3)
Cd(1)-O(12)	2.309(3)
Cd(1)-O(5)#3	2.223(3)
Cd(1)-O(6)#2	2.349(3)
Cd(2)-N(4)	2.274(3)
Cd(2)-N(5)	2.333(4)
Cd(2)-O(2)	2.227(3)
Cd(2)-OW3	2.378(3)
Cd(2)-O(8)#1	2.301(3)
Cd(2)-O(7)#1	2.432(3)
Cd(3)-N(8)	2.216(3)
Cd(3)-N(9)	2.283(4)
Cd(3)-O(3)#4	2.299(3)
Cd(3)-O(4)#4	2.340(3)
Cd(3)-O(9)	2.234(3)
O(5)#3-Cd(1)-N(12)	85.26(12)
O(5)#3-Cd(1)-N(1)	120.10(12)
N(12)-Cd(1)-N(1)	149.67(13)
O(5)#3-Cd(1)-O(12)	90.58(14)
N(12)-Cd(1)-O(12)	108.14(13)
N(1)-Cd(1)-O(12)	89.26(13)
O(5)#3-Cd(1)-O(6)#2	94.24(10)
N(12)-Cd(1)-O(6)#2	83.60(11)
N(1)-Cd(1)-O(6)#2	78.50(10)
O(12)-Cd(1)-O(6)#2	167.67(12)
O(2)-Cd(2)-N(4)	92.58(12)
O(2)-Cd(2)-O(8)#1	113.07(10)
N(4)-Cd(2)-O(8)#1	152.99(11)
O(2)-Cd(2)-N(5)	85.98(12)
N(4)-Cd(2)-N(5)	104.72(13)
O(8)#1-Cd(2)-N(5)	86.15(12)
O(2)-Cd(2)-OW3	89.95(10)
N(4)-Cd(2)-OW3	85.74(11)
O(8)#1-Cd(2)-OW3	85.97(10)
N(5)-Cd(2)-OW3	168.92(11)
O(2)-Cd(2)-O(7)#1	166.41(10)
N(4)-Cd(2)-O(7)#1	100.00(11)
O(8)#1-Cd(2)-O(7)#1	55.49(9)
N(5)-Cd(2)-O(7)#2	85.87(11)
OW3-Cd(2)-O(7)#1	96.04(10)

N(8)-Cd(3)-O(9)	106.31(13)
N(8)-Cd(3)-N(9)	110.70(13)
O(9)-Cd(3)-N(9)	86.53(13)
N(8)-Cd(3)-O(3)#4	150.38(12)
O(9)-Cd(3)-O(3)#4	97.37(12)
N(9)-Cd(3)-O(3)#4	87.88(13)
N(8)-Cd(3)-O(4)#4	94.49(12)
O(9)-Cd(3)-O(4)#4	145.82(13)
N(9)-Cd(3)-O(4)#4	111.46(13)
O(3)#4-Cd(3)-O(4)#4	56.50(10)
N(8)-Cd(3)-O(10)	86.64(12)
O(9)-Cd(3)-O(10)	53.49(12)
N(9)-Cd(3)-O(10)	139.89(12)
O(3)#4-Cd(3)-O(10)	93.62(12)
O(4)#4-Cd(3)-O(10)	102.43(12)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+1,-z+2; #2 -x-1,-y,-z+1; #3 x-1,y,z; #4 x-1,y+1,z.