

Electronic Supplementary Information

Synthesis, Crystal Structure, and Luminescence Properties of Seven Tripodal Imidazole-based Zn/Cd(II) Coordination Polymers Induced by Tricarboxylates

Wei Yang, Chiming Wang, Qi Ma, Chenxi Liu, Hailong Wang, and Jianzhuang

Jiang*

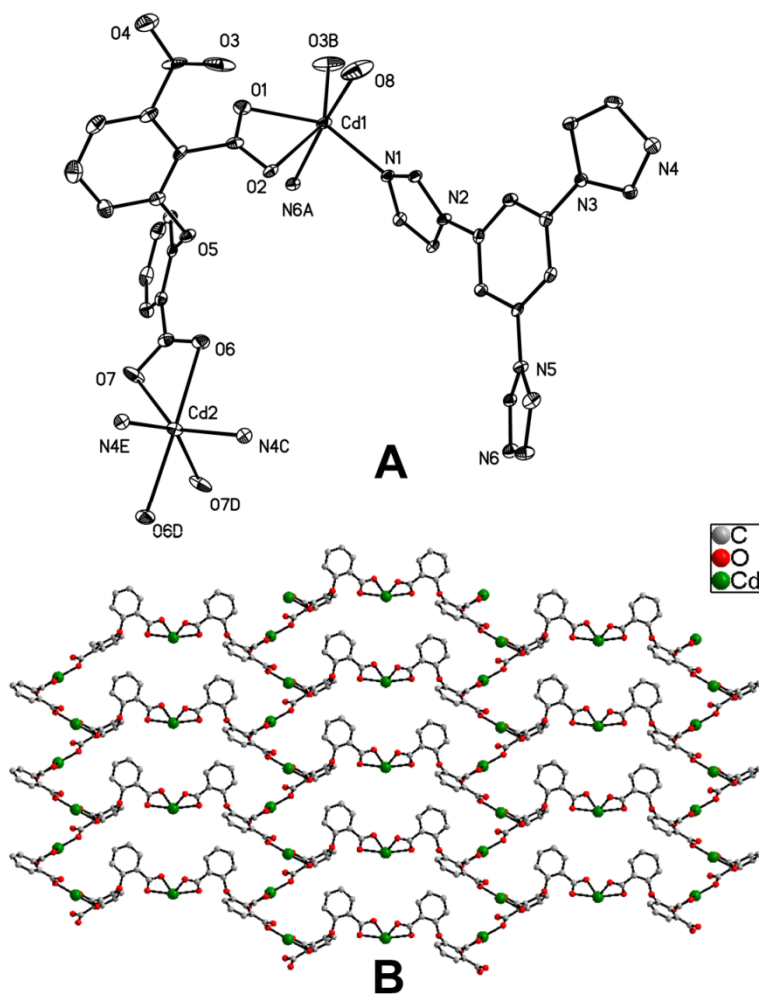


Figure S1. (A) The coordination geometry for Cd(II) atoms in **2** with the 30% probability level, all hydrogen atoms and solvent water molecules have been omitted for clarity. (B) 2D sheet in **2**. [Symmetry codes: (i) $1 - x, -y, 2 - z$ for N6A; (ii) $0.5 - x, -0.5 + y, 1.5 - z$ for O3B; (iii) $1 - x, 1 - y, 2 - z$ for N4C; (iv) $1 - x, y, 2.5 - z$ for O6D and O6D; (v) $x, 1 - y, 0.5 + z$ for N4E]

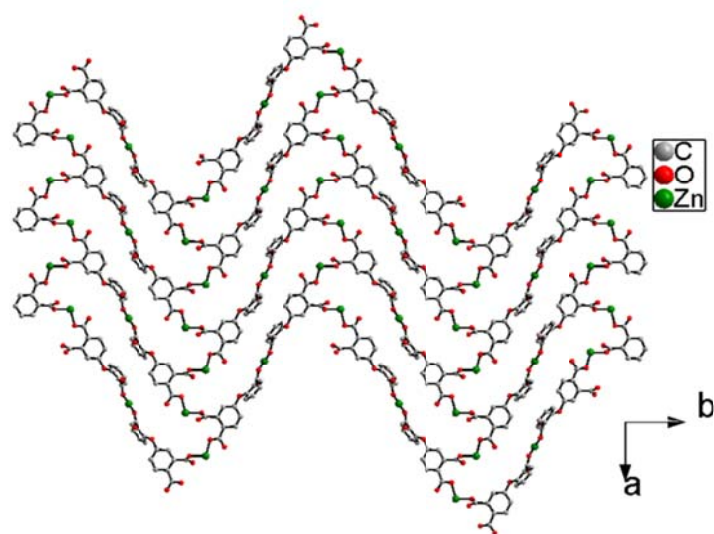


Figure S2. A 2D wavy sheet in **3**.

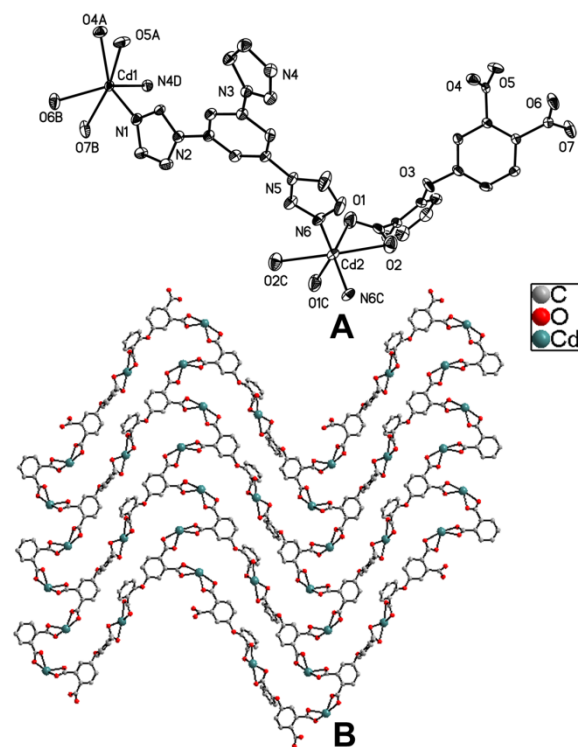


Figure S3. (A) The coordination geometry for Cd(II) atoms in **4** with the 30% probability level, all hydrogen atoms and solvent water molecules have been omitted for clarity. (B) 2D sheet in **4**. [Symmetry codes: (i) $1 - x, -1.5 + y, 0.5 - z$ for O4A and O5A; (ii) $x, -2 + y, z$ for O6B and O7B; (iii) $1.5 - x, 1.5 - y, z$ for O1C, O2C, and N6C; (iv) $x, 0.5 - y, -0.5 - z$ for N4D]

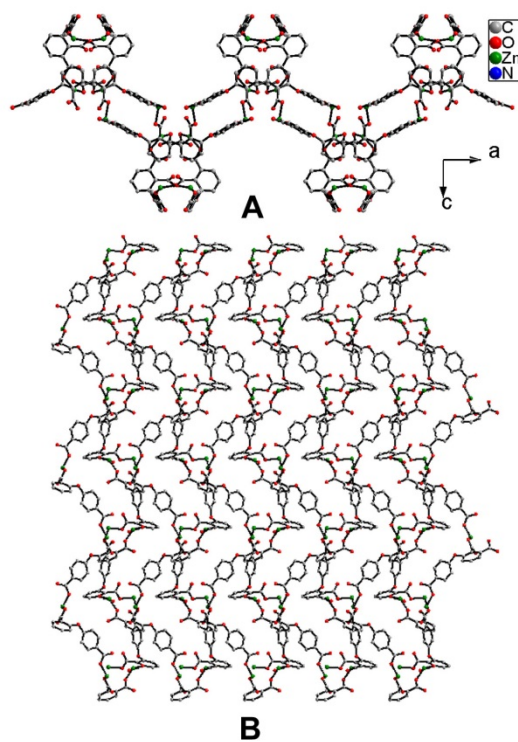


Figure S4. 2D wavy sheet in **5** in the view of *b* axis (A) and *c* axis (B).

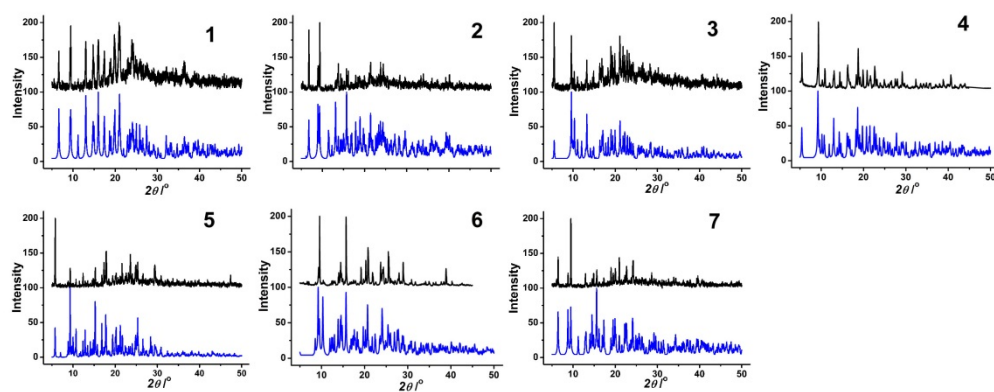


Figure S5. Powder X-ray diffraction pattern of 1-7 (black for recorded curve and blue for simulated curve).

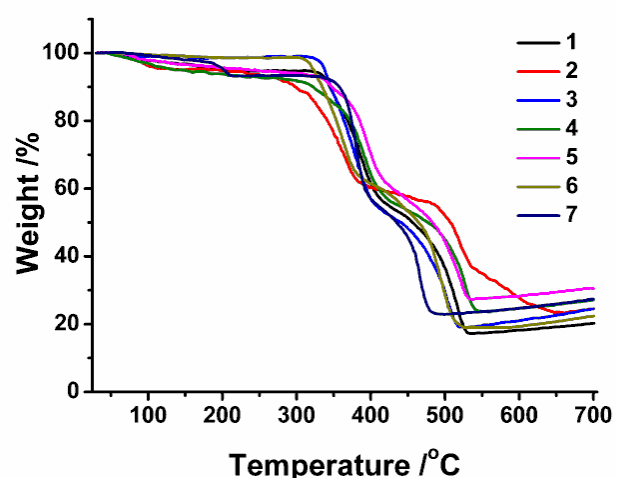


Figure S6. The TGA curves of **1-7** in the range of 30-700°C in the air.

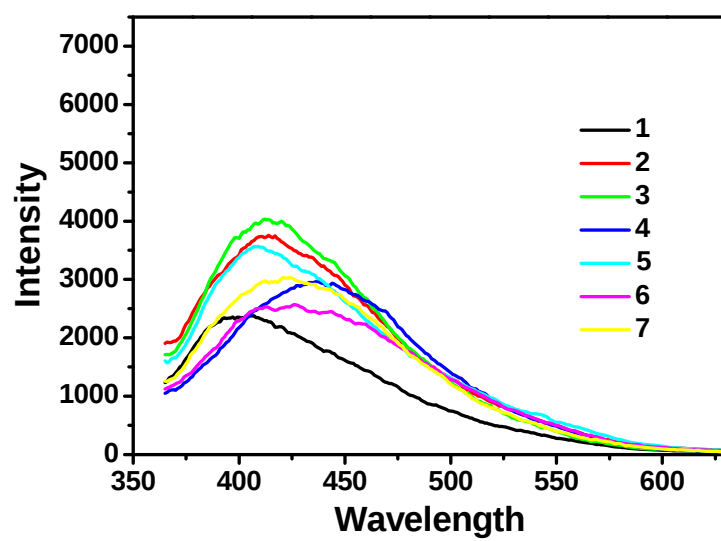


Figure S7. Luminescence emission band of compounds **1-7**.

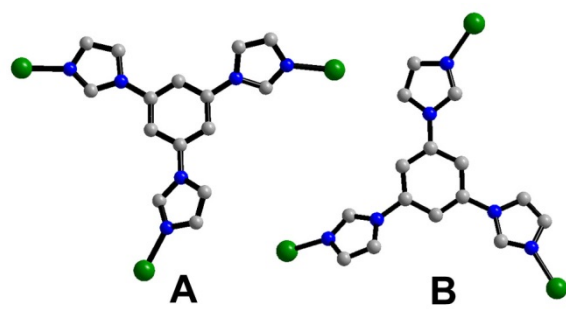


Figure S8. Mode A for 1, 5, 6, and 7 and mode B for 2, 3, and 4.

Table S1. Selected bond distances (Å) and bond angles (°)

Complex 1			
N(1)-Zn(1)	2.024(5)	Zn(1)-N(1)#4	2.024(5)
N(3)-Zn(2)	2.033(6)	Zn(1)-O(6)#5	2.122(5)
N(6)-Zn(2)#2	2.020(5)	Zn(1)-O(6)#6	2.122(5)
O(2)-Zn(2)	1.979(4)	Zn(1)-O(7)#5	2.298(7)
O(3)-Zn(2)#3	2.103(5)	Zn(1)-O(7)#6	2.298(7)
O(4)-Zn(2)#3	2.485(6)	Zn(2)-N(6)#2	2.020(5)
O(6)-Zn(1)#1	2.122(5)	Zn(2)-O(3)#7	2.103(5)
O(7)-Zn(1)#1	2.298(7)	Zn(2)-O(4)#7	2.485(6)
N(1)#4-Zn(1)-O(6)#5	104.4(2)	O(6)#6-Zn(1)-O(7)#6	57.81(19)
N(1)-Zn(1)-O(6)#5	94.5(2)	O(7)#5-Zn(1)-O(7)#6	91.0(3)
N(1)#4-Zn(1)-O(6)#6	94.5(2)	O(2)-Zn(2)-N(6)#2	113.5(2)
N(1)-Zn(1)-O(6)#6	104.4(2)	O(2)-Zn(2)-N(3)	100.9(2)
O(6)#5-Zn(1)-O(6)#6	152.6(3)	N(6)#2-Zn(2)-N(3)	116.4(2)
N(1)#4-Zn(1)-O(7)#5	94.5(2)	O(2)-Zn(2)-O(3)#7	97.5(2)
N(1)-Zn(1)-O(7)#5	152.3(2)	N(6)#2-Zn(2)-O(3)#7	106.9(2)
O(6)#5-Zn(1)-O(7)#5	57.81(19)	N(3)-Zn(2)-O(3)#7	119.9(2)
O(6)#6-Zn(1)-O(7)#5	101.6(2)	O(2)-Zn(2)-O(4)#7	148.36(19)
N(1)#4-Zn(1)-O(7)#6	152.3(2)	N(6)#2-Zn(2)-O(4)#7	91.4(2)
N(1)-Zn(1)-O(7)#6	94.5(2)	N(3)-Zn(2)-O(4)#7	83.6(2)
O(6)#5-Zn(1)-O(7)#6	101.6(2)	O(3)#7-Zn(2)-O(4)#7	54.9(2)
Complex 2			
N(1)-Cd(1)	2.310(4)	O(8)-Cd(1)	2.344(5)
N(6)-Cd(1)#2	2.358(5)	Cd(1)-O(3)#4	2.210(5)
O(1)-Cd(1)	2.300(4)	Cd(1)-N(6)#2	2.358(5)
O(2)-Cd(1)	2.592(4)	Cd(2)-N(4)#1	2.249(5)
O(3)-Cd(1)#3	2.210(4)	Cd(2)-N(4)#5	2.249(5)
O(6)-Cd(2)	2.429(4)	Cd(2)-O(7)#6	2.287(5)
O(7)-Cd(2)	2.287(5)	Cd(2)-O(6)#6	2.429(4)
O(3)#4-Cd(1)-O(1)	94.9(2)	N(4)#1-Cd(2)-N(4)#5	88.0(2)
O(3)#4-Cd(1)-N(1)	127.3(2)	N(4)#1-Cd(2)-O(7)	143.01(16)
O(1)-Cd(1)-N(1)	137.65(15)	N(4)#5-Cd(2)-O(7)	98.44(18)
O(3)#4-Cd(1)-O(8)	91.4(2)	N(4)#1-Cd(2)-O(7)#6	98.44(18)
O(1)-Cd(1)-O(8)	93.84(19)	N(4)#5-Cd(2)-O(7)#6	143.01(16)
N(1)-Cd(1)-O(8)	82.75(17)	O(7)-Cd(2)-O(7)#6	97.8(3)
O(3)#4-Cd(1)-N(6)#2	99.59(18)	N(4)#1-Cd(2)-O(6)#6	102.56(16)
O(1)-Cd(1)-N(6)#2	85.53(16)	N(4)#5-Cd(2)-O(6)#6	87.79(16)

N(1)-Cd(1)-N(6)#2	90.35(16)	O(7)-Cd(2)-O(6)#6	114.00(16)
O(8)-Cd(1)-N(6)#2	169.06(18)	O(7)#6-Cd(2)-O(6)#6	55.23(15)
O(3)#4-Cd(1)-O(2)	148.2(2)	N(4)#1-Cd(2)-O(6)	87.79(16)
O(1)-Cd(1)-O(2)	53.42(12)	N(4)#5-Cd(2)-O(6)	102.56(16)
N(1)-Cd(1)-O(2)	84.26(14)	O(7)-Cd(2)-O(6)	55.23(15)
O(8)-Cd(1)-O(2)	89.05(18)	O(7)#6-Cd(2)-O(6)	114.00(16)
N(6)#2-Cd(1)-O(2)	81.79(14)	O(6)#6-Cd(2)-O(6)	165.7(2)

Complex 3

O(1)-Zn(1)#1	1.985(7)	Zn(2)-O(7)#5	1.854(14)
O(3)-Zn(1)	1.957(8)	Zn(2)-O(7)#6	1.854(14)
O(7)-Zn(2)#2	1.854(14)	Zn(2)-N(3)	1.999(9)
Zn(1)-O(1)#3	1.985(7)	Zn(2)-N(3)#7	1.999(9)
Zn(1)-N(1)	2.018(8)	N(6)-Zn(1)#8	2.061(8)
Zn(1)-N(6)#4	2.061(8)		

O(3)-Zn(1)-O(1)#3	105.2(3)	O(7)#5-Zn(2)-O(7)#6	85.6(9)
O(3)-Zn(1)-N(1)	117.3(3)	O(7)#5-Zn(2)-N(3)	111.1(5)
O(1)#3-Zn(1)-N(1)	118.2(3)	O(7)#6-Zn(2)-N(3)	124.4(5)
O(3)-Zn(1)-N(6)#4	99.2(3)	O(7)#5-Zn(2)-N(3)#7	124.4(5)
O(1)#3-Zn(1)-N(6)#4	117.9(3)	O(7)#6-Zn(2)-N(3)#7	111.1(5)
N(1)-Zn(1)-N(6)#4	97.8(3)	N(3)-Zn(2)-N(3)#7	101.8(5)

Complex 4

N(1)-Cd(1)	2.232(4)	Cd(1)-O(4)#4	2.251(4)
N(6)-Cd(2)	2.218(4)	Cd(1)-N(4)#5	2.290(5)
O(1)-Cd(2)	2.277(5)	Cd(1)-O(6)#6	2.312(4)
O(2)-Cd(2)	2.505(5)	Cd(1)-O(7)#6	2.438(4)
O(4)-Cd(1)#2	2.251(4)	Cd(1)-O(5)#4	2.542(4)
O(5)-Cd(1)#2	2.542(4)	Cd(2)-N(6)#7	2.218(4)
O(6)-Cd(1)#3	2.312(4)	Cd(2)-O(1)#7	2.277(5)
O(7)-Cd(1)#3	2.438(4)	Cd(2)-O(2)#7	2.505(5)

N(1)-Cd(1)-O(4)#4	135.76(16)	N(6)#7-Cd(2)-N(6)	93.7(2)
N(1)-Cd(1)-N(4)#5	96.73(17)	N(6)#7-Cd(2)-O(1)#7	101.3(2)
O(4)#4-Cd(1)-N(4)#5	93.27(17)	N(6)-Cd(2)-O(1)#7	144.85(18)
N(1)-Cd(1)-O(6)#6	106.02(19)	N(6)#7-Cd(2)-O(1)	144.85(18)
O(4)#4-Cd(1)-O(6)#6	97.03(17)	N(6)-Cd(2)-O(1)	101.3(2)
N(4)#5-Cd(1)-O(6)#6	134.10(16)	O(1)#7-Cd(2)-O(1)	84.3(3)
N(1)-Cd(1)-O(7)#6	94.48(18)	N(6)#7-Cd(2)-O(2)#7	109.59(18)
O(4)#4-Cd(1)-O(7)#6	129.24(17)	N(6)-Cd(2)-O(2)#7	91.45(18)
N(4)#5-Cd(1)-O(7)#6	85.87(16)	O(1)#7-Cd(2)-O(2)#7	53.62(17)
O(6)#6-Cd(1)-O(7)#6	53.60(14)	O(1)-Cd(2)-O(2)#7	101.67(19)
N(1)-Cd(1)-O(5)#4	82.50(15)	N(6)#7-Cd(2)-O(2)	91.45(18)

O(4)#4-Cd(1)-O(5)#4	53.86(14)	N(6)-Cd(2)-O(2)	109.59(18)
N(4)#5-Cd(1)-O(5)#4	111.28(16)	O(1)#7-Cd(2)-O(2)	101.67(19)
O(6)#6-Cd(1)-O(5)#4	110.84(16)	O(1)-Cd(2)-O(2)	53.62(17)
O(7)#6-Cd(1)-O(5)#4	162.79(16)	O(2)#7-Cd(2)-O(2)	149.4(3)

Complex 5

O(2)-Zn(2)	2.026(4)	Zn(1)-N(1)	2.053(5)
O(3)-Zn(1)#1	1.933(4)	Zn(2)-O(7)#7	1.950(4)
O(7)-Zn(2)#2	1.950(4)	Zn(2)-N(7)	2.000(4)
O(8)-Zn(3)#1	1.928(4)	Zn(2)-N(4)	2.026(5)
O(11)-Zn(1)#3	1.952(4)	Zn(3)-O(8)#4	1.928(4)
O(13)-Zn(3)	1.927(4)	Zn(3)-N(10)	1.980(5)
Zn(1)-O(3)#4	1.933(4)	Zn(3)-N(12)#8	2.009(5)
Zn(1)-O(11)#5	1.952(4)	N(6)-Zn(1)#9	2.019(5)
Zn(1)-N(6)#6	2.019(5)	N(12)-Zn(3)#8	2.009(5)
O(3)#4-Zn(1)-O(11)#5	126.52(19)	O(7)#7-Zn(2)-O(2)	105.31(17)
O(3)#4-Zn(1)-N(6)#6	102.11(19)	N(7)-Zn(2)-O(2)	119.22(18)
O(11)#5-Zn(1)-N(6)#6	107.9(2)	N(4)-Zn(2)-O(2)	106.15(18)
O(3)#4-Zn(1)-N(1)	103.71(19)	O(13)-Zn(3)-O(8)#4	103.8(2)
O(11)#5-Zn(1)-N(1)	105.20(19)	O(13)-Zn(3)-N(10)	116.7(2)
N(6)#6-Zn(1)-N(1)	111.1(2)	O(8)#4-Zn(3)-N(10)	109.2(2)
O(7)#7-Zn(2)-N(7)	111.94(18)	O(13)-Zn(3)-N(12)#8	100.7(2)
O(7)#7-Zn(2)-N(4)	95.58(18)	O(8)#4-Zn(3)-N(12)#8	111.4(2)
N(7)-Zn(2)-N(4)	115.7(2)	N(10)-Zn(3)-N(12)#8	114.5(2)

Complex 6

N(9)-Zn(2)#1	2.013(7)	O(1)-Zn(1)	1.975(6)
N(1)-Zn(1)	2.043(7)	O(9)-Zn(2)	1.979(6)
N(3)-Zn(2)	2.034(7)	Zn(1)-N(6)#4	1.970(6)
N(7)-Zn(2)	2.014(7)	Zn(1)-N(11)#5	2.028(7)
N(11)-Zn(1)#2	2.028(7)	Zn(2)-N(9)#6	2.013(7)
N(6)-Zn(1)#3	1.970(6)		
N(6)#4-Zn(1)-O(1)	123.7(3)	O(9)-Zn(2)-N(9)#6	124.4(3)
N(6)#4-Zn(1)-N(11)#5	104.6(3)	O(9)-Zn(2)-N(7)	120.3(3)
O(1)-Zn(1)-N(11)#5	120.9(3)	N(9)#6-Zn(2)-N(7)	100.3(3)
N(6)#4-Zn(1)-N(1)	105.5(3)	O(9)-Zn(2)-N(3)	99.0(3)
O(1)-Zn(1)-N(1)	93.7(3)	N(9)#6-Zn(2)-N(3)	107.5(3)
N(11)#5-Zn(1)-N(1)	105.0(3)	N(7)-Zn(2)-N(3)	102.8(3)

Complex 7

O(1)-Cd(1)	2.340(6)	Cd(1)-N(1)	2.341(6)
O(2)-Cd(1)	2.476(8)	Cd(1)-O(4)#3	2.650(5)

O(3)-Cd(1)#2	2.290(4)	Cd(2)-N(4)#5	2.249(7)
O(4)-Cd(1)#2	2.650(5)	Cd(2)-N(4)	2.249(7)
O(6)-Cd(2)#1	2.456(6)	Cd(2)-O(7)#6	2.281(6)
O(7)-Cd(2)#1	2.281(6)	Cd(2)-O(7)#7	2.281(6)
O(9)-Cd(1)	2.306(6)	Cd(2)-O(6)#6	2.456(6)
Cd(1)-O(3)#3	2.290(4)	Cd(2)-O(6)#7	2.456(6)
Cd(1)-N(6)#4	2.316(6)	N(6)-Cd(1)#8	2.316(6)
O(3)#3-Cd(1)-O(9)	94.6(3)	O(1)-Cd(1)-O(4)#3	135.1(2)
O(3)#3-Cd(1)-N(6)#4	138.0(2)	N(1)-Cd(1)-O(4)#3	82.30(19)
O(9)-Cd(1)-N(6)#4	84.3(3)	O(2)-Cd(1)-O(4)#3	172.7(2)
O(3)#3-Cd(1)-O(1)	83.2(2)	N(4)#5-Cd(2)-N(4)	91.2(4)
O(9)-Cd(1)-O(1)	94.5(3)	N(4)#5-Cd(2)-O(7)#6	102.9(3)
N(6)#4-Cd(1)-O(1)	138.8(2)	N(4)-Cd(2)-O(7)#6	141.0(2)
O(3)#3-Cd(1)-N(1)	85.6(2)	N(4)#5-Cd(2)-O(7)#7	141.0(2)
O(9)-Cd(1)-N(1)	172.8(3)	N(4)-Cd(2)-O(7)#7	102.9(3)
N(6)#4-Cd(1)-N(1)	90.6(2)	O(7)#6-Cd(2)-O(7)#7	88.6(4)
O(1)-Cd(1)-N(1)	92.7(2)	N(4)#5-Cd(2)-O(6)#6	102.3(2)
O(3)#3-Cd(1)-O(2)	135.3(2)	N(4)-Cd(2)-O(6)#6	88.0(2)
O(9)-Cd(1)-O(2)	86.5(3)	O(7)#6-Cd(2)-O(6)#6	53.7(2)
N(6)#4-Cd(1)-O(2)	86.7(2)	O(7)#7-Cd(2)-O(6)#6	114.1(2)
O(1)-Cd(1)-O(2)	52.2(2)	N(4)#5-Cd(2)-O(6)#7	88.0(2)
N(1)-Cd(1)-O(2)	98.4(3)	N(4)-Cd(2)-O(6)#7	102.3(2)
O(3)#3-Cd(1)-O(4)#3	51.98(17)	O(7)#6-Cd(2)-O(6)#7	114.1(2)
O(9)-Cd(1)-O(4)#3	92.2(3)	O(7)#7-Cd(2)-O(6)#7	53.7(2)
N(6)#4-Cd(1)-O(4)#3	86.0(2)	O(6)#6-Cd(2)-O(6)#7	165.3(3)

Symmetry transformations used to generate equivalent atoms: For **1**, #1: x,y-1,z; #2: -x+1,-y+1,-z; #3: -x+3/2,y-1/2,-z+1/2; #4: -x+1,y,-z-1/2; #5: x,y+1,z; #6: -x+1,y+1,-z-1/2; #7: -x+3/2,y+1/2,-z+1/2. For **2**, #1: -x+1,-y+1,-z+2; #2: -x+1,-y,-z+2; #3: -x+1/2,y+1/2,-z+3/2; #4: -x+1/2,y-1/2,-z+3/2; #5: x,-y+1,z+1/2; #6: -x+1,y,-z+5/2. For **3**, #1: x-1/2,-y,-z+1/2; #2: x+3/2,-y,-z+1/2; #3: x+1/2,-y,-z+1/2; #4: -x-1/2,y,z-1/2; #5: x-3/2,-y,-z+1/2; #6: -x,y+1/2,-z+1/2; #7: -x-3/2,-y+1/2,z; #8: -x-1/2,y,z+1/2. For **4**, #1: x,-y+1/2,z+1/2; #2: -x+1,y+3/2,-z+1/2; #3: x,y+2,z; #4: -x+1,y-3/2,-z+1/2; #5: x,-y+1/2,z-1/2; #6: x,y-2,z; #7: -x+3/2,-y+3/2,z. For **5**, #1: -x+3/2,y+1/2,z; #2: -x+1,y-1/2,-z+1/2; #3: -x+3/2,-y+3,z+1/2; #4: -x+3/2,y-1/2,z; #5: -x+3/2,-y+3,z-1/2; #6: x+1/2,y,-z+1/2; #7: -x+1,y+1/2,-z+1/2; #8: -x+2,-y+3,-z+1; #9: x-1/2,y,-z+1/2. For **6**, #1: x,y-1,z; #2: x,y,z-1; #3: x-1,y+1,z; #4: x+1,y-1,z; #5: x,y,z+1; #6: x,y+1,z. For **7**, #1: x+1/2,y-3/2,z-1; #2: -x+3/2,y-1/2,-z-1; #3: -x+3/2,y+1/2,-z-1; #4: -x+1,y+1,-z-1; #5: -x+1,y,-z; #6: -x+3/2,y+3/2,-z-1; #7: x-1/2,y+3/2,z+1; #8: -x+1,y-1,-z-1.