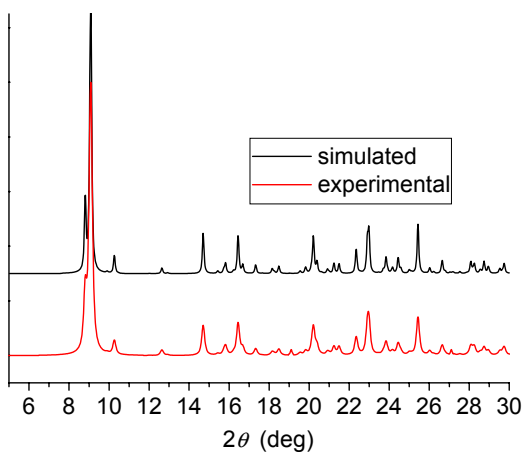


Electronic Supplementary Information

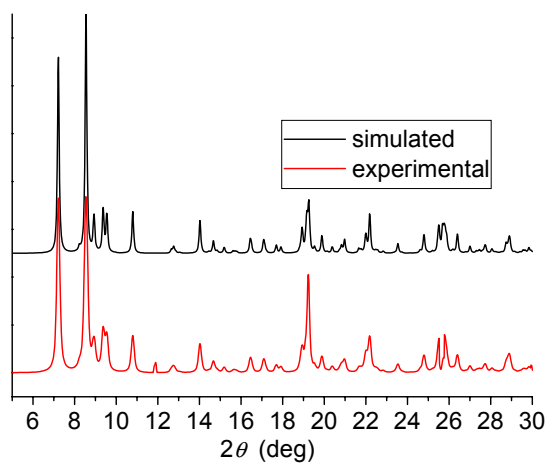
d¹⁰ Metal Complexes Assembled from Isomeric Benzenedicarboxylates and 3-(2-Pyridyl)pyrazole Showing 1D Structures: Syntheses, Structures and Luminescent Properties

Tong-Liang Hu, Ruo-Qiang Zou, Jian-Rong Li and Xian-He Bu^{*}

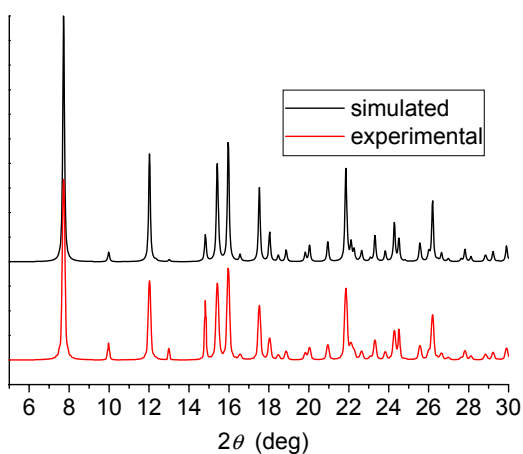
Department of Chemistry, Nankai University, Tianjin 300071, China



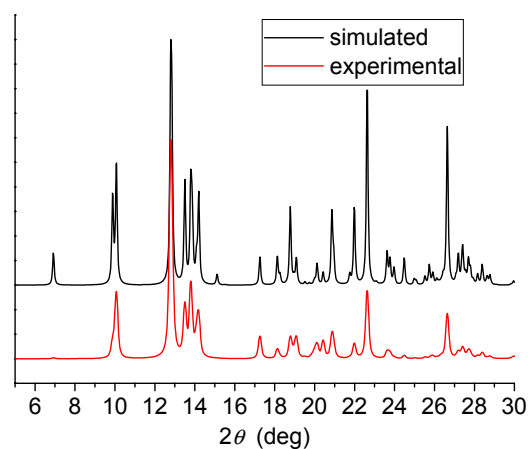
(a)



(b)



(c)



(d)

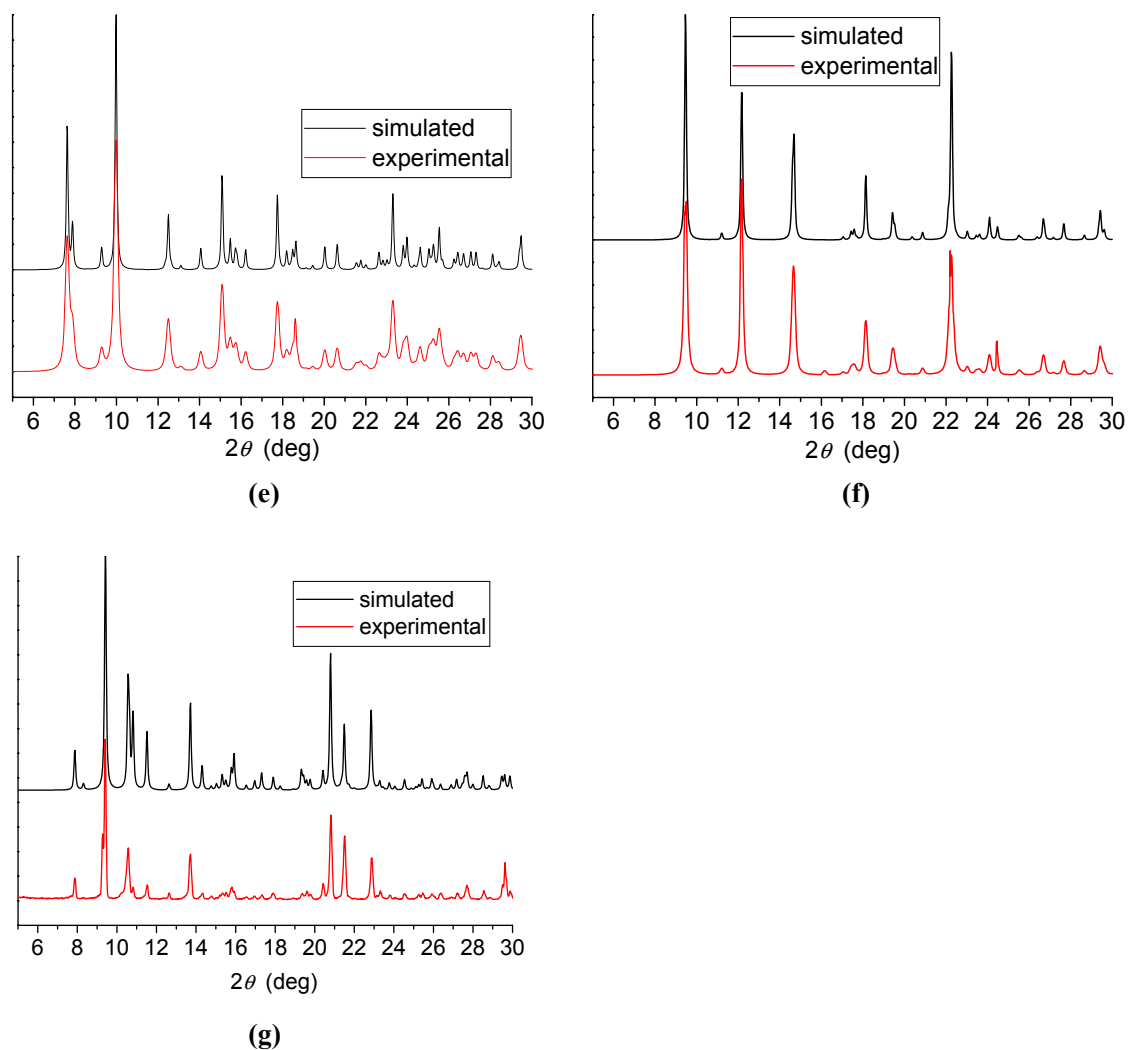
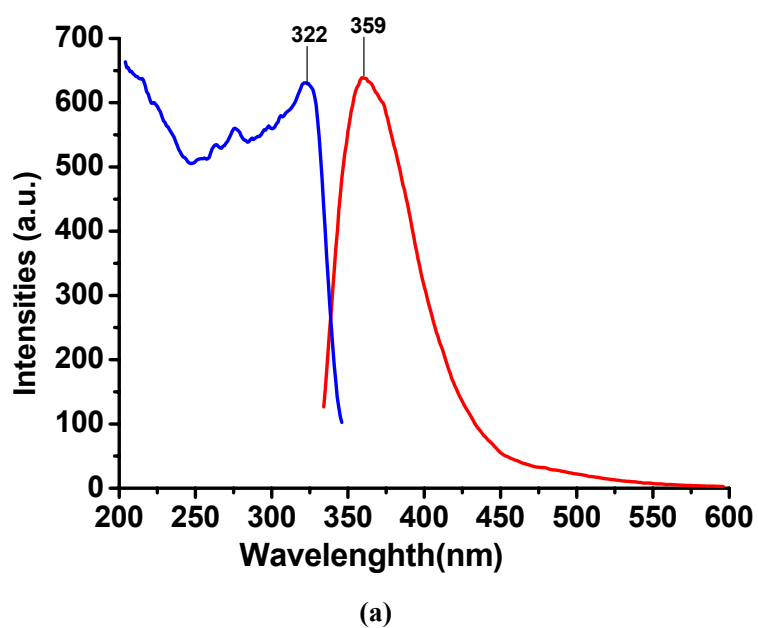
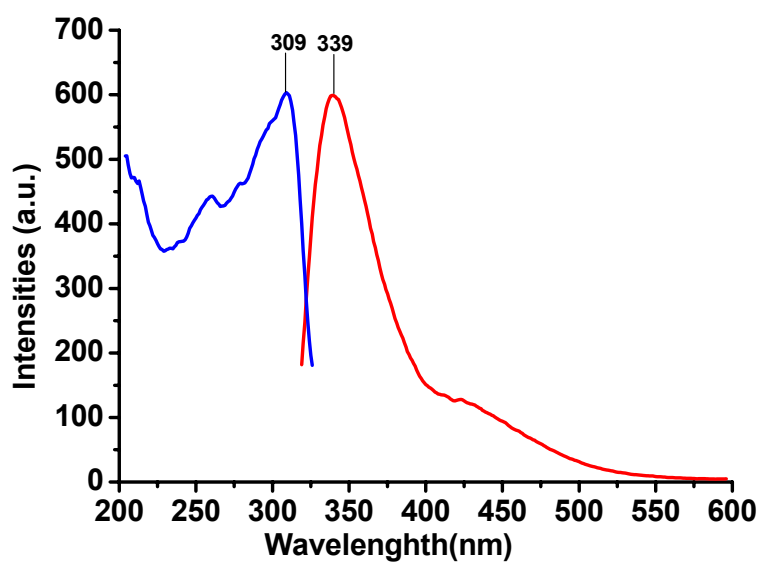
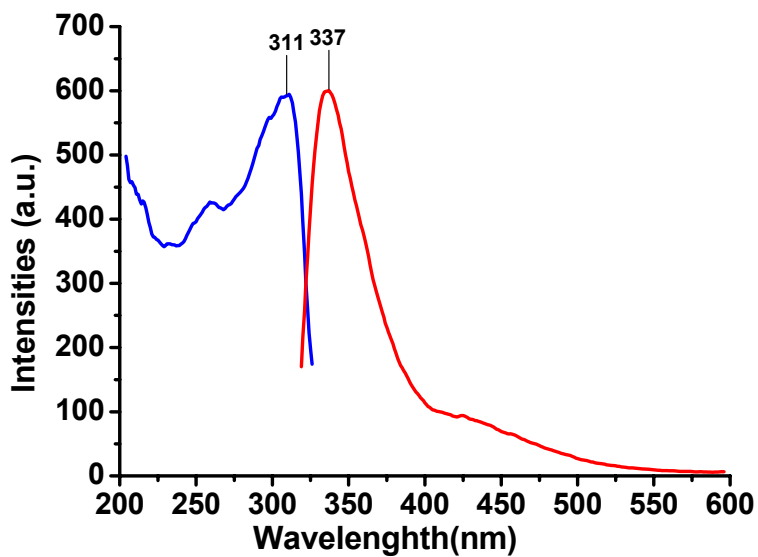


Fig. S1 XRPD patterns of complexes **1-7**: (a) for **1**, (b) for **2**, (c) for **3**, (d) for **4**, (e) for **5**, (f) for **6**, and (g) for **7**.

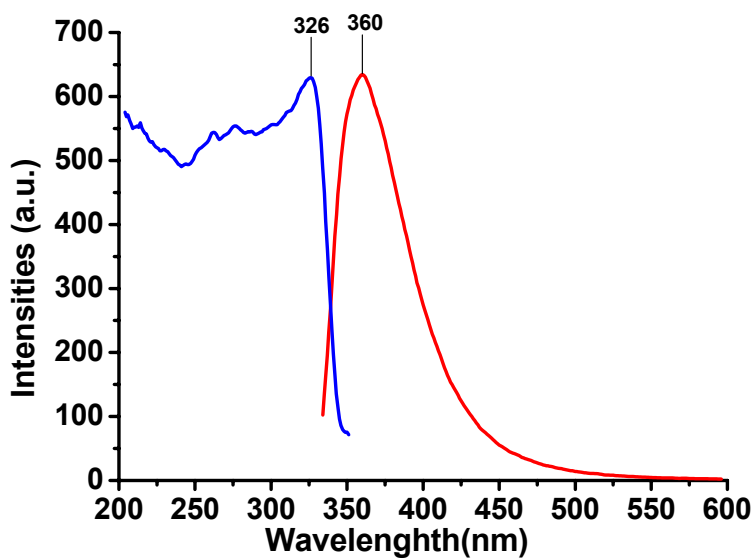




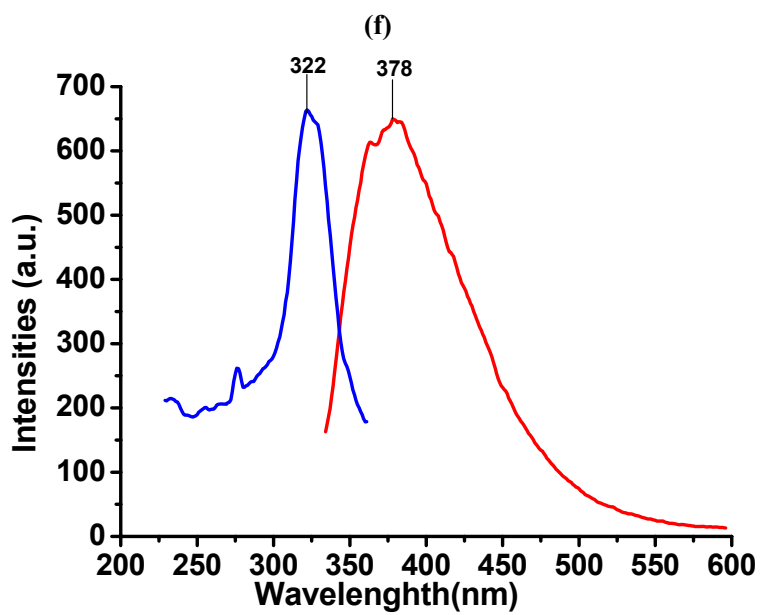
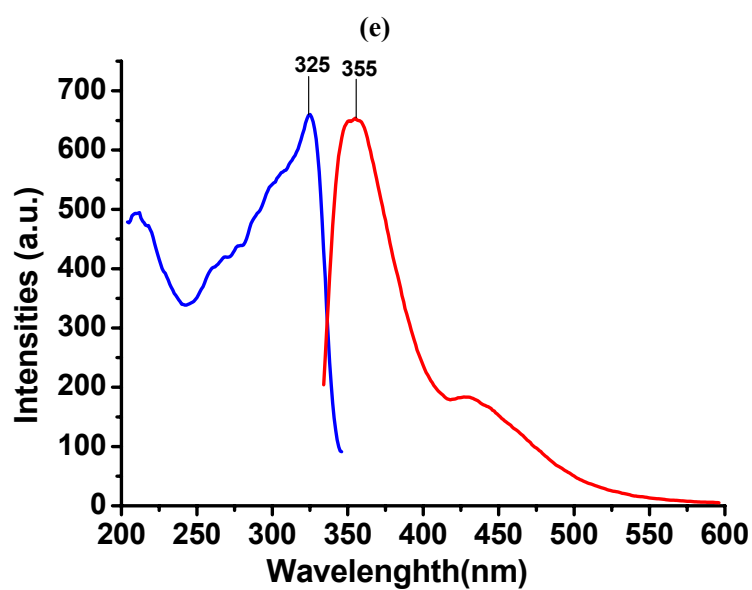
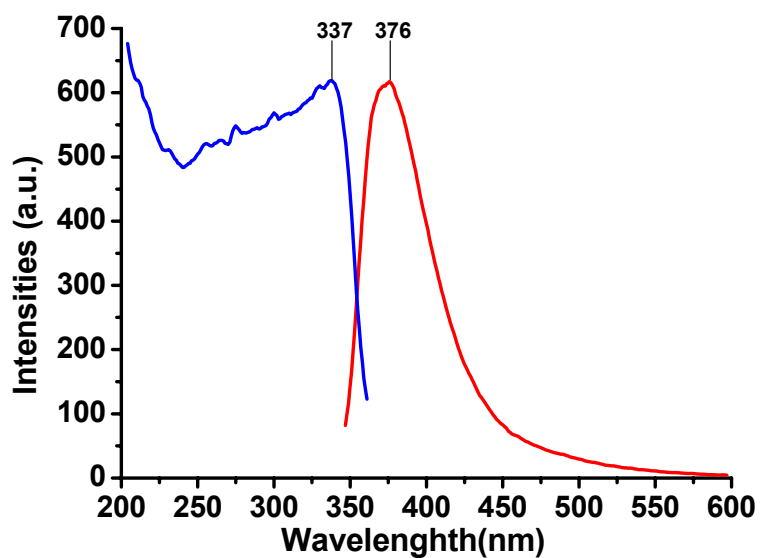
(b)



(c)



(d)



(g)

Fig. S2 Excitation and emission spectra of 1-7 in the solid state at room temperature: (a) for 1, (b) for 2, (c) for 3, (d) for 4, (e) for 5, (f) for 6, and (g) for 7.

Table S1. Selected bond lengths [Å] and angles [°] for complexes **1-7**

1			
Zn(1)-N(5)	2.234(7)	Zn(1)-N(2)	2.256(7)
Zn(1)-O(3)	2.340(6)	Zn(1)-N(4)	2.364(7)
Zn(1)-N(1)	2.387(8)	Zn(1)-O(3)#1	2.399(6)
Zn(2)-N(3)	2.245(7)	Zn(2)-N(6)	2.253(7)
Zn(2)-O(4)	2.302(6)	Zn(2)-O(2)	2.405(8)
Zn(2)-O(1)	2.460(8)	Zn(2)-O(1W)	2.473(8)
N(5)-Zn(1)-N(2)	161.3(3)	N(5)-Zn(1)-O(3)	106.7(2)
N(2)-Zn(1)-O(3)	90.5(2)	N(5)-Zn(1)-N(4)	72.4(2)
N(2)-Zn(1)-N(4)	100.0(3)	O(3)-Zn(1)-N(4)	93.1(2)
N(5)-Zn(1)-N(1)	93.3(3)	N(2)-Zn(1)-N(1)	71.5(3)
O(3)-Zn(1)-N(1)	157.4(2)	N(4)-Zn(1)-N(1)	103.1(3)
N(5)-Zn(1)-O(3)#1	93.6(2)	N(2)-Zn(1)-O(3)#1	97.2(2)
O(3)-Zn(1)-O(3)#1	78.1(2)	N(4)-Zn(1)-O(3)#1	160.7(2)
N(1)-Zn(1)-O(3)#1	90.5(2)	N(3)-Zn(2)-N(6)	93.5(3)
N(3)-Zn(2)-O(4)	124.2(2)	N(6)-Zn(2)-O(4)	101.7(2)
N(3)-Zn(2)-O(2)	89.9(2)	N(6)-Zn(2)-O(2)	107.8(3)
O(4)-Zn(2)-O(2)	133.0(3)	N(3)-Zn(2)-O(1)	142.4(2)
N(6)-Zn(2)-O(1)	88.6(3)	O(4)-Zn(2)-O(1)	91.9(2)
O(2)-Zn(2)-O(1)	54.1(2)	N(3)-Zn(2)-O(1W)	89.0(3)
N(6)-Zn(2)-O(1W)	177.5(3)	O(4)-Zn(2)-O(1W)	76.7(2)
O(2)-Zn(2)-O(1W)	72.3(3)	O(1)-Zn(2)-O(1W)	89.6(2)
2			
Cd(1)-N(2)	2.267(3)	Cd(1)-O(2)	2.309(3)
Cd(1)-O(3)	2.319(3)	Cd(1)-O(5)	2.379(3)
Cd(1)-N(1)	2.427(3)	Cd(1)-O(3)#1	2.445(3)
Cd(1)-O(4)	2.581(3)	Cd(2)-O(6)	2.218(3)
Cd(2)-O(7)	2.306(3)	Cd(2)-N(4)	2.323(3)
Cd(2)-O(1)	2.392(3)	Cd(2)-N(5)	2.433(4)
Cd(2)-O(2)	2.458(3)		
N(2)-Cd(1)-O(2)	95.76(1)	N(2)-Cd(1)-O(3)	152.60(1)

O(2)-Cd(1)-O(3)	100.96(9)	N(2)-Cd(1)-O(5)	81.03(1)
O(2)-Cd(1)-O(5)	83.62(9)	O(3)-Cd(1)-O(5)	79.45(9)
N(2)-Cd(1)-N(1)	69.49(1)	O(2)-Cd(1)-N(1)	122.59(1)
O(3)-Cd(1)-N(1)	117.17(1)	O(5)-Cd(1)-N(1)	141.43(1)
N(2)-Cd(1)-O(3)#1	132.83(1)	O(2)-Cd(1)-O(3)#1	75.42(9)
O(3)-Cd(1)-O(3)#1	72.98(1)	O(5)-Cd(1)-O(3)#1	141.06(1)
N(1)-Cd(1)-O(3)#1	76.83(1)	N(2)-Cd(1)-O(4)	105.41(1)
O(2)-Cd(1)-O(4)	151.42(9)	O(3)-Cd(1)-O(4)	52.57(9)
O(5)-Cd(1)-O(4)	81.03(1)	N(1)-Cd(1)-O(4)	83.39(1)
O(3)#1-Cd(1)-O(4)	102.36(1)	O(6)-Cd(2)-O(7)	93.86(1)
O(6)-Cd(2)-N(4)	97.70(1)	O(7)-Cd(2)-N(4)	115.76(1)
O(6)-Cd(2)-O(1)	145.61(1)	O(7)-Cd(2)-O(1)	85.83(1)
N(4)-Cd(2)-O(1)	113.39(1)	O(6)-Cd(2)-N(5)	92.56(1)
O(7)-Cd(2)-N(5)	171.23(1)	N(4)-Cd(2)-N(5)	69.16(1)
O(1)-Cd(2)-N(5)	85.49(1)	O(6)-Cd(2)-O(2)	91.91(1)
O(7)-Cd(2)-O(2)	92.91(9)	N(4)-Cd(2)-O(2)	148.85(1)
O(1)-Cd(2)-O(2)	53.84(9)	N(5)-Cd(2)-O(2)	80.91(1)

3

Cd(1)-O(3)	2.243(5)	Cd(1)-O(2)	2.247(4)
Cd(1)-N(2)	2.290(5)	Cd(1)-O(1W)	2.299(4)
Cd(1)-N(1)	2.321(5)	Cd(1)-O(4)	2.575(4)
O(3)-Cd(1)-O(2)	82.80(2)	O(3)-Cd(1)-N(2)	166.5(2)
O(2)-Cd(1)-N(2)	106.66(2)	O(3)-Cd(1)-O(1W)	98.6(2)
O(2)-Cd(1)-O(1W)	104.03(2)	N(2)-Cd(1)-O(1W)	88.63(2)
O(3)-Cd(1)-N(1)	98.0(2)	O(2)-Cd(1)-N(1)	101.02(2)
N(2)-Cd(1)-N(1)	71.01(2)	O(1W)-Cd(1)-N(1)	151.40(2)
O(3)-Cd(1)-O(4)	52.71(2)	O(2)-Cd(1)-O(4)	134.57(1)
N(2)-Cd(1)-O(4)	118.76(2)	O(1W)-Cd(1)-O(4)	77.47(2)
N(1)-Cd(1)-O(4)	94.56(2)		

4

Zn(1)-O(3)#1	2.0067(2)	Zn(1)-N(1)	2.122(2)
Zn(1)-O(1W)	2.133(2)	Zn(1)-O(2)	2.166(3)
Zn(1)-N(2)	2.168(2)	Zn(1)-O(1)	2.331(2)
O(3)#1-Zn(1)-N(1)	122.81(9)	O(3)#1-Zn(1)-O(1W)	89.17(9)
N(1)-Zn(1)-O(1W)	90.88(1)	O(3)#1-Zn(1)-O(2)	91.01(8)
N(1)-Zn(1)-O(2)	146.14(9)	O(1W)-Zn(1)-O(2)	91.46(1)
O(3)#1-Zn(1)-N(2)	97.12(8)	N(1)-Zn(1)-N(2)	77.14(9)
O(1W)-Zn(1)-N(2)	168.01(1)	O(2)-Zn(1)-N(2)	98.59(9)
O(3)#1-Zn(1)-O(1)	148.77(9)	N(1)-Zn(1)-O(1)	88.29(9)
O(1W)-Zn(1)-O(1)	93.48(9)	O(2)-Zn(1)-O(1)	57.85(9)
N(2)-Zn(1)-O(1)	86.44(9)		

5

Cd(1)-N(6)	2.233(3)	Cd(1)-O(1)#1	2.258(3)
Cd(1)-O(1W)	2.304(3)	Cd(1)-N(2)	2.319(3)
Cd(1)-N(1)	2.325(3)	Cd(2)-N(3)	2.223(3)
Cd(2)-N(5)	2.255(3)	Cd(2)-N(4)	2.357(3)
Cd(2)-O(3)	2.371(2)	Cd(2)-O(3)#2	2.421(3)
Cd(2)-O(4)	2.500(3)		
N(6)-Cd(1)-O(1)#1	87.54(12)	N(6)-Cd(1)-O(1W)	98.96(12)
O(1)#1-Cd(1)-O(1W)	120.24(14)	N(6)-Cd(1)-N(2)	96.82(11)
O(1)#1-Cd(1)-N(2)	144.99(13)	O(1W)-Cd(1)-N(2)	93.48(11)
N(6)-Cd(1)-N(1)	152.78(11)	O(1)#1-Cd(1)-N(1)	88.39(12)
O(1W)-Cd(1)-N(1)	106.31(12)	N(2)-Cd(1)-N(1)	72.04(11)
N(3)-Cd(2)-N(5)	98.67(11)	N(3)-Cd(2)-N(4)	148.89(11)
N(5)-Cd(2)-N(4)	72.28(11)	N(3)-Cd(2)-O(3)	101.99(11)
N(5)-Cd(2)-O(3)	137.60(10)	N(4)-Cd(2)-O(3)	104.33(10)
N(3)-Cd(2)-O(3)#2	87.40(10)	N(5)-Cd(2)-O(3)#2	145.90(9)
N(4)-Cd(2)-O(3)#2	85.23(10)	O(3)-Cd(2)-O(3)#2	72.01(9)
N(3)-Cd(2)-O(4)	102.82(10)	N(5)-Cd(2)-O(4)	86.33(10)
N(4)-Cd(2)-O(4)	106.11(10)	O(3)-Cd(2)-O(4)	53.20(8)
O(3)#2-Cd(2)-O(4)	125.21(8)		

6

Zn(1)-O(1)	2.068(2)	Zn(1)-N(2)	2.089(2)
Zn(1)-N(1)	2.327(2)		
O(1)#1-Zn(1)-O(1)	97.62(1)	O(1)-Zn(1)-N(2)#1	98.71(7)
O(1)-Zn(1)-N(2)	96.93(7)	N(2)#1-Zn(1)-N(2)	156.15(1)
O(1)-Zn(1)-N(1)#1	89.55(8)	N(2)-Zn(1)-N(1)#1	89.40(7)
O(1)-Zn(1)-N(1)	168.40(7)	N(2)#1-Zn(1)-N(1)	89.40(7)
N(2)-Zn(1)-N(1)	72.88(7)	N(1)#1-Zn(1)-N(1)	84.91(1)

7

Cd(1)-O(3)	2.259(2)	Cd(1)-N(5)	2.387(3)
Cd(1)-O(1)	2.427(2)	Cd(1)-O(2)	2.447(3)
Cd(1)-N(4)	2.454(3)	Cd(1)-N(2)	2.455(3)
Cd(1)-N(1)	2.457(3)		
O(3)-Cd(1)-N(5)	111.95(8)	O(3)-Cd(1)-O(1)	96.45(8)
N(5)-Cd(1)-O(1)	128.75(9)	O(3)-Cd(1)-O(2)	86.63(9)
N(5)-Cd(1)-O(2)	85.54(9)	O(1)-Cd(1)-O(2)	53.45(8)
O(3)-Cd(1)-N(4)	178.62(1)	N(5)-Cd(1)-N(4)	68.05(9)
O(1)-Cd(1)-N(4)	84.51(1)	O(2)-Cd(1)-N(4)	94.74(1)
O(3)-Cd(1)-N(2)	97.67(9)	N(5)-Cd(1)-N(2)	138.10(9)
O(1)-Cd(1)-N(2)	73.15(9)	O(2)-Cd(1)-N(2)	126.53(9)
N(4)-Cd(1)-N(2)	81.64(10)	O(3)-Cd(1)-N(1)	86.42(9)
N(5)-Cd(1)-N(1)	85.17(9)	O(1)-Cd(1)-N(1)	140.28(9)
O(2)-Cd(1)-N(1)	165.40(9)	N(4)-Cd(1)-N(1)	92.20(1)
N(2)-Cd(1)-N(1)	67.22(9)		

Symmetry mode: **1**, -x+1,-y,-z; **3**, -x+1,-y+2,-z+1; **4**, x,y+1,z; **5**, #1 x,y-1,z, #2- x,-y+2,-z+1; **6**, #1 -x,y,-z+1/2