Electronic Supplementary Information (ESI) for CEC

Assembly of A Series of d^{10} Coordination Polymers Based on W-shaped 1,3-Di(2',4'-dicarboxylphenyl)benzene: From Syntheses, Structural Diversity, Luminescence, to Photocatalytic Properties

Xiutang Zhang,*[a,b] Liming Fan,[a,b] Weiliu Fan,[b] Bin Li[a] and Xian Zhao*[b]

[a] *Advanced Material Institute of Research, College of Chemistry and Chemical Engineering, Qilu Normal University, Jinan, 250013, China.*
[b] *State Key Laboratory of Crystal Materials, Shandong University , Jinan 250100, China.*

E-mail: xiutangzhang@163.com (X.Z.); zhaoxian@sdu.edu.cn (X. Zhao).

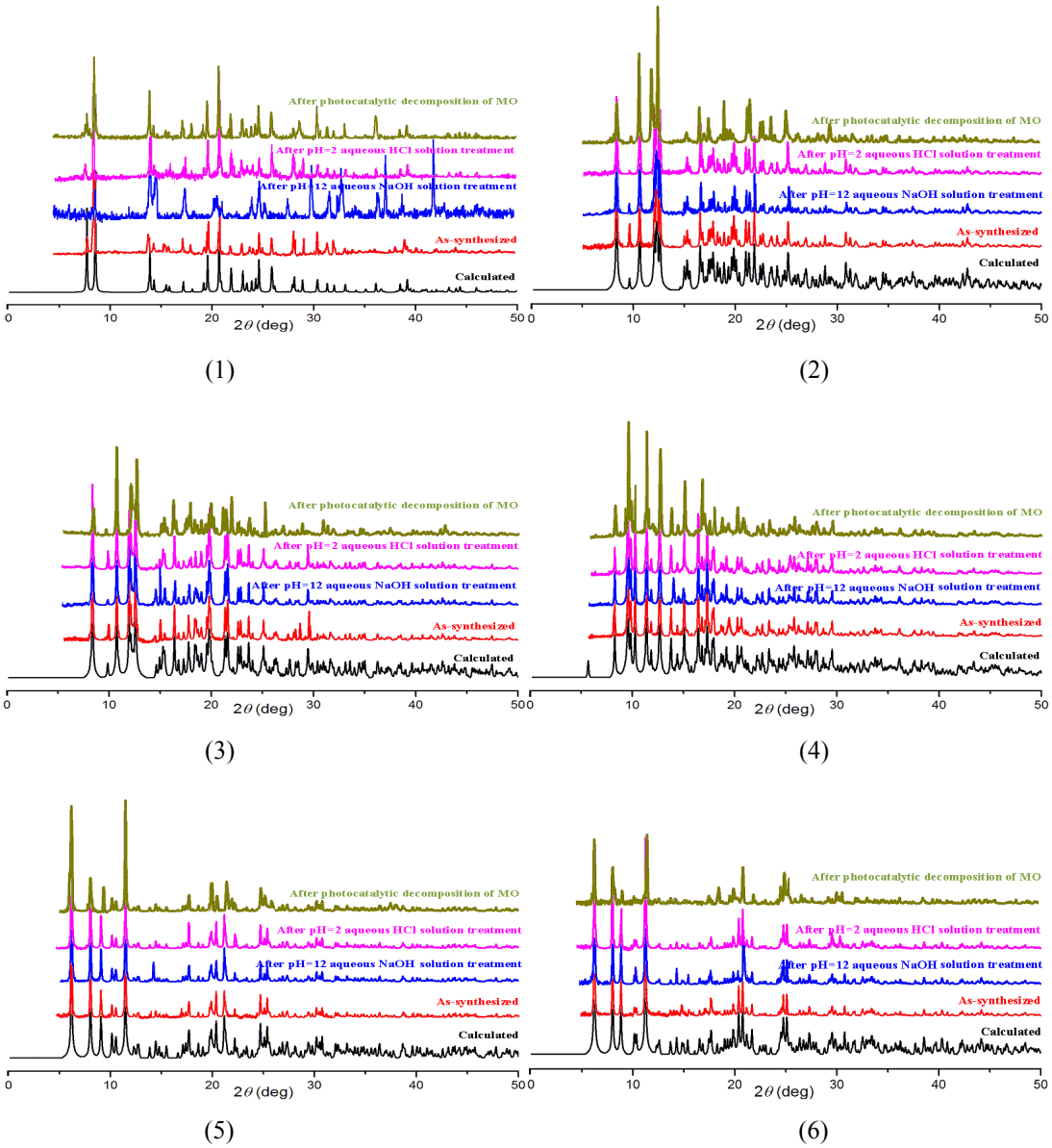
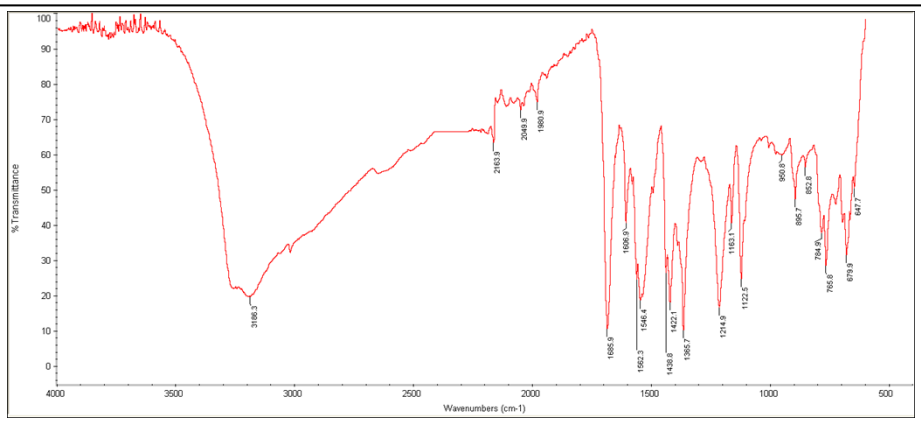
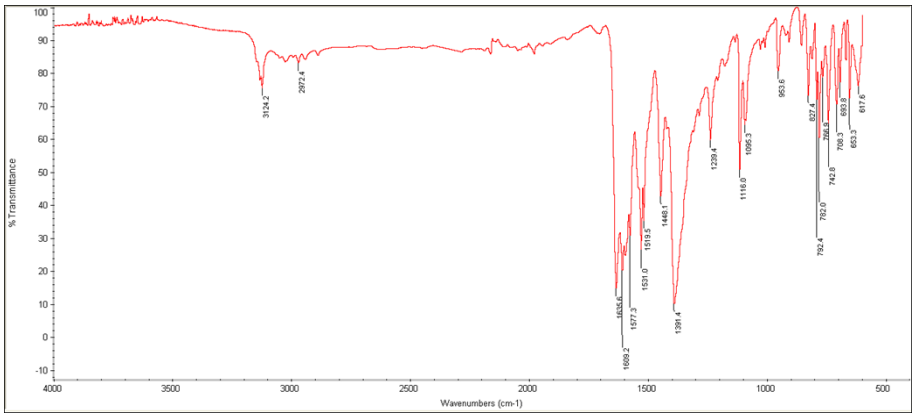


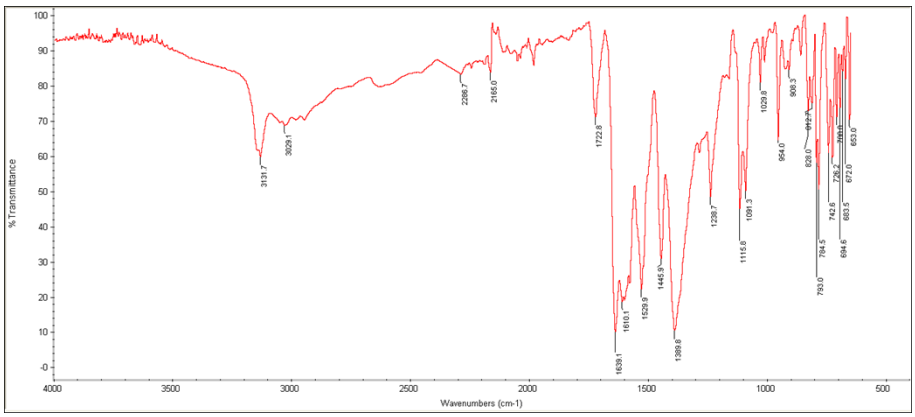
Figure S1. PXRD patterns of complexes **1-6** under different conditions treatment.


% Transmittance
Wavenumbers (cm-1)
3186.3
2163.9
2049.8
1980.9
1685.9
1698.9
1562.3
1546.4
1438.8
1422.1
1365.7
1214.9
1163.1
1122.5
950.6
895.7
852.8
784.9
765.6
679.9
647.7

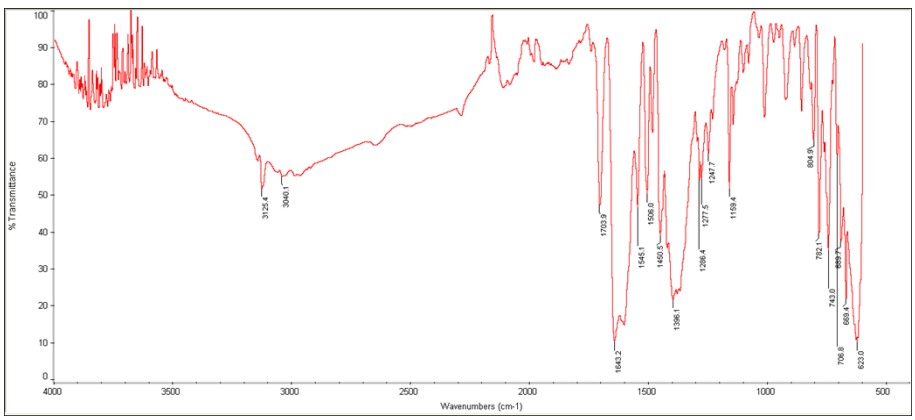
(1)


% Transmittance
Wavenumbers (cm-1)
3124.2
2972.4
1669.2
1634.4
1577.3
1531.0
1515.5
1448.1
1391.4
1239.4
1116.0
1095.3
953.6
827.4
792.4
792.0
742.8
708.3
693.9
653.3
617.6

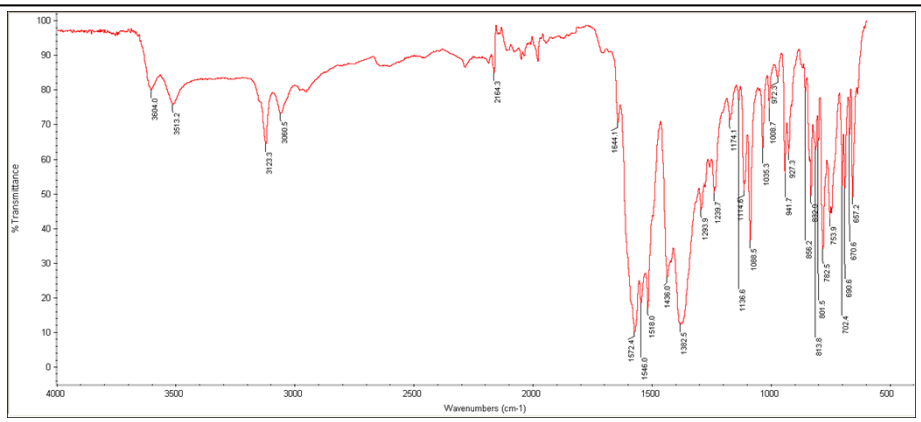
(2)


% Transmittance
Wavenumbers (cm-1)
3131.7
3029.1
2286.7
2165.0
1722.8
1638.1
1610.1
1529.9
1445.8
1389.8
1239.7
1115.6
1091.3
1029.8
954.0
908.3
828.0
793.0
784.5
742.6
694.6
683.5
672.0
653.0

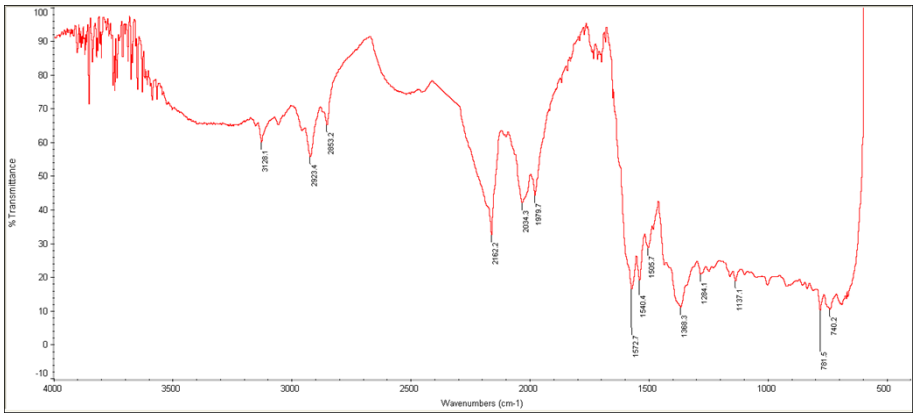
(3)


% Transmittance
Wavenumbers (cm-1)
3125.4
3040.1
1710.9
1643.2
1606.0
1545.1
1460.5
1396.1
1286.4
1277.5
1247.7
1159.4
804.9
762.1
743.0
706.8
689.4
623.0

(4)



(5)



(6)

Figure S2. The IR spectras of complexes **1**-**6**.

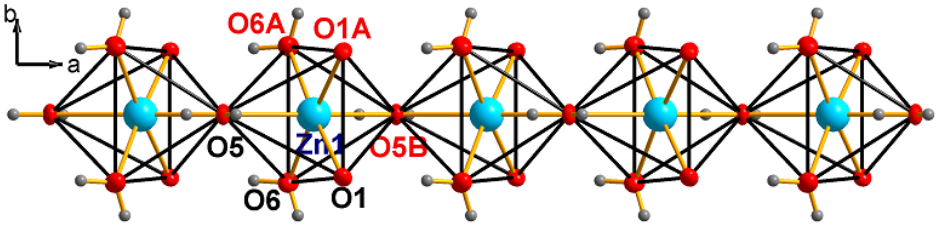


Figure S3. The water molecules bridged 1D chain view along *c* direction.

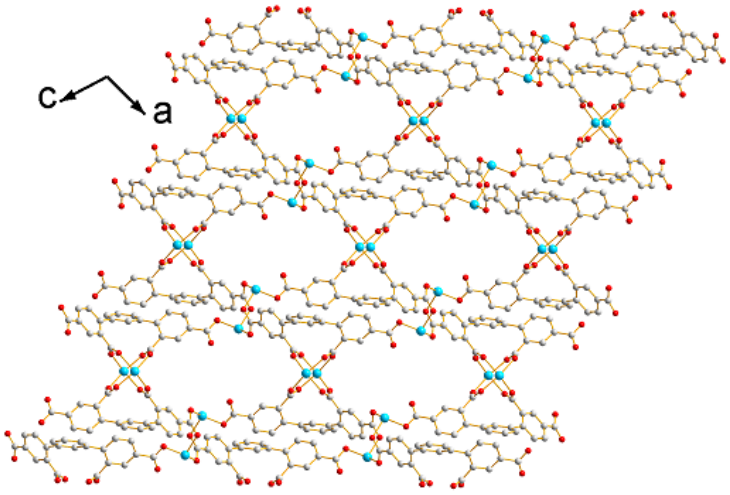


Figure S4. The 3D $[Zn_2(DDB)]_n$ net view along *b* axis in complex **2**.

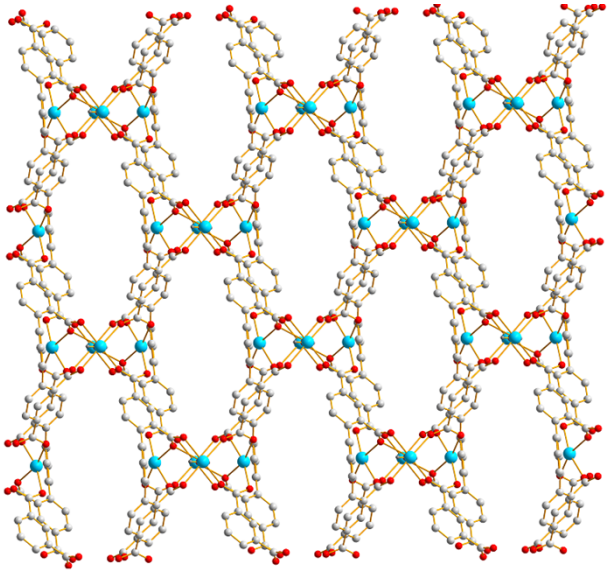


Figure S5. The 3D $[Cd_2(DDB)]_n$ net view along *b* axis in complex **5**.

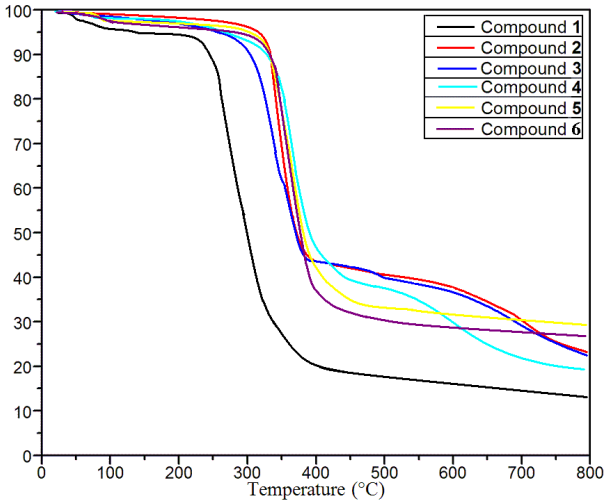


Figure S6. TGA curves for compounds **1**−**6**.

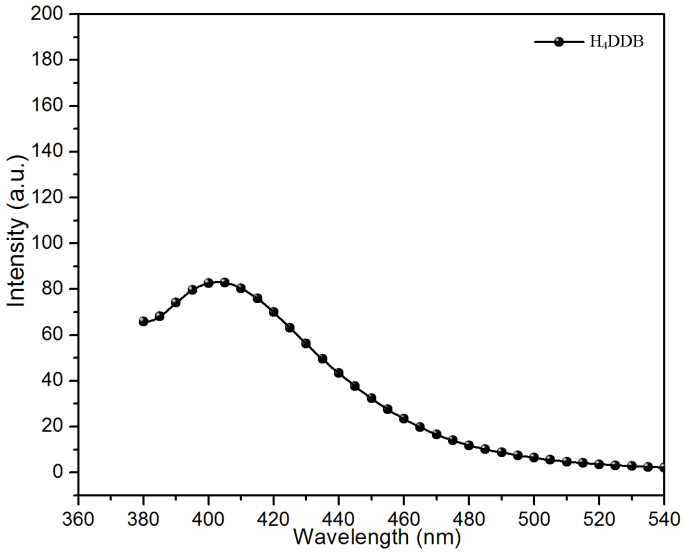


Figure S7. Emissions pectra of H_4DDB in the solid state at room temperature.

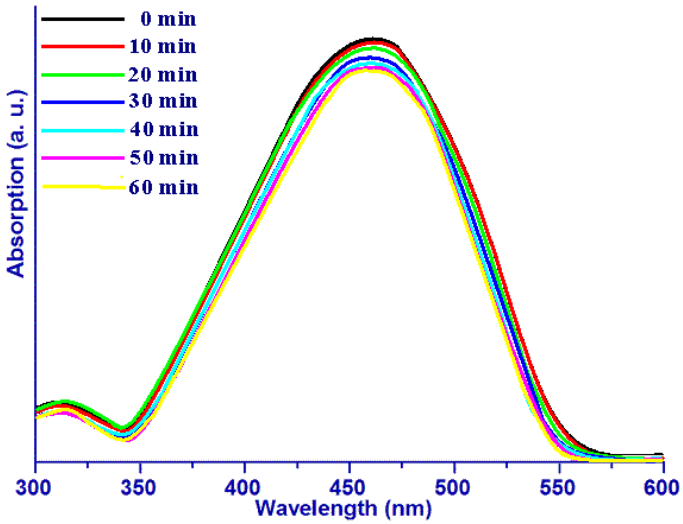


Figure S8. UV-Vis absorption spectra of the MO solutions degraded without photocatalysts.

Table S1 Selected bond lengths (Å) and angles (°) for **1** –**6**.

Complex **1**							
Zn(1)-O(6)	2.0406(17)	Zn(1)-O(1)	2.0808(16)	Zn(1)-O(5)	2.152(2)	O(6)$^{\#1}$-Zn(1)-O(5)	87.51(7)
O(6)-Zn(1)-O(6)$^{\#1}$	96.04(10)	O(6)$^{\#1}$-Zn(1)-O(1)	174.26(7)	O(1)$^{\#1}$-Zn(1)-O(5)$^{\#2}$	93.67(7)	O(1)$^{\#1}$-Zn(1)-O(5)	93.12(7)
O(6)-Zn(1)-O(1)$^{\#1}$	174.26(7)	O(1)$^{\#1}$-Zn(1)-O(1)	84.58(9)	O(1)-Zn(1)-O(5)$^{\#2}$	93.67(7)	O(1)-Zn(1)-O(5)	93.12(7)
O(6)$^{\#1}$-Zn(1)-O(1)$^{\#1}$	89.69(7)	O(6)-Zn(1)-O(5)$^{\#2}$	86.35(7)	O(6)-Zn(1)-O(5)	87.51(7)	O(5)$^{\#2}$-Zn(1)-O(5)	170.81(6)
O(6)-Zn(1)-O(1)	89.69(7)	O(6)$^{\#1}$-Zn(1)-O(5)$^{\#2}$	86.35(7)	O(1)$^{\#1}$-Zn(1)-O(5)$^{\#2}$	93.67(7)		
Symmetry codes: #1 *x*, -*y*+3/2, *z*; #2 *x*+1/2, *y*, -*z*+1/2.							
Complex **2**							
N(1)-Zn(2)	1.992(5)	O(5)-Zn(1)	2.046(3)	Zn(1)-O(3)$^{\#2}$	2.066(3)	Zn(2)-O(7)$^{\#5}$	1.970(4)
O(2)-Zn(2)	1.963(3)	Zn(1)-N(4)$^{\#1}$	1.984(4)	Zn(1)-O(6)$^{\#2}$	2.059(3)	Zn(2)-O(8)$^{\#6}$	2.077(3)
O(4)-Zn(1)	2.029(3)	O(2)-Zn(2)-N(1)	109.17(17)	N(4)$^{\#1}$-Zn(1)-O(4)	102.97(15)	N(4)$^{\#1}$-Zn(1)-O(5)	102.02(15)
O(4)-Zn(1)-O(5)	87.49(14)	O(4)-Zn(1)-O(3)$^{\#2}$	158.96(14)	O(5)-Zn(1)-Zn(1)$^{\#2}$	72.45(10)	O(7)$^{\#5}$-Zn(2)-N(1)	108.26(17)
N(4)$^{\#1}$-Zn(1)-O(6)$^{\#2}$	98.91(15)	O(5)-Zn(1)-O(3)$^{\#2}$	89.18(14)	O(6)$^{\#2}$-Zn(1)-Zn(1)$^{\#2}$	86.59(10)	O(2)-Zn(2)-O(8)$^{\#6}$	95.27(14)
O(4)-Zn(1)-O(6)$^{\#2}$	89.09(15)	O(6)$^{\#2}$-Zn(1)-O(3)$^{\#2}$	86.63(15)	O(3)$^{\#2}$-Zn(1)-Zn(1)$^{\#2}$	80.04(10)	O(7)$^{\#5}$-Zn(2)-O(8)$^{\#6}$	104.19(14)
O(5)-Zn(1)-O(6)$^{\#2}$	159.03(14)	N(4)$^{\#1}$-Zn(1)-Zn(1)$^{\#2}$	174.09(11)	O(2)-Zn(2)-O(7)$^{\#5}$	133.81(17)	N(1)-Zn(2)-O(8)$^{\#6}$	99.59(16)
N(4)$^{\#1}$-Zn(1)-O(3)$^{\#2}$	98.04(15)	O(4)-Zn(1)-Zn(1)$^{\#2}$	79.15(10)				
Symmetry codes: #1 -*x*+2, -*y*+1, -*z*+2; #2 -*x*+2, -*y*+2, -*z*+2; #3 *x*-1/2, -*y*+5/2, *z*+1/2; #4 -*x*+3/2, *y*+1/2, -*z*+3/2; #5 *x*+1/2, -*y*+5/2, *z*-1/2; #6 -*x*+3/2, *y*-1/2, -*z*+3/2.							
Complex **3**							
N(1)-Zn(1)	1.991(4)	O(7)-Zn(1)	2.082(3)	Zn(1)-O(1)$^{\#2}$	2.046(3)	Zn(2)-N(4)$^{\#6}$	2.001(4)
O(2)-Zn(1)	2.050(3)	Zn(1)-O(8)$^{\#2}$	2.030(3)	Zn(2)-O(3)$^{\#5}$	1.982(3)	Zn(2)-O(4)$^{\#7}$	2.071(3)
O(6)-Zn(2)	1.972(3)	N(1)-Zn(1)-O(8)$^{\#2}$	104.96(16)	N(1)-Zn(1)-O(1)$^{\#2}$	99.83(15)	O(8)$^{\#2}$-Zn(1)-O(1)$^{\#2}$	88.10(13)
N(1)-Zn(1)-O(2)	101.82(15)	O(8)$^{\#2}$-Zn(1)-O(7)	158.52(13)	O(6)-Zn(2)-O(3)$^{\#5}$	135.39(15)	O(6)-Zn(2)-O(4)$^{\#7}$	93.28(13)
O(8)$^{\#2}$-Zn(1)-O(2)	88.68(13)	O(1)$^{\#2}$-Zn(1)-O(7)	88.21(13)	O(6)-Zn(2)-N(4)$^{\#6}$	109.51(16)	O(3)$^{\#5}$-Zn(2)-O(4)$^{\#7}$	105.74(13)
O(1)$^{\#2}$-Zn(1)-O(2)	158.21(13)	O(2)-Zn(1)-O(7)	86.94(13)	O(3)$^{\#5}$-Zn(2)-N(4)$^{\#6}$	104.77(17)	N(4)$^{\#6}$-Zn(2)-O(4)$^{\#7}$	103.43(15)
N(1)-Zn(1)-O(7)	96.52(16)						
Symmetry codes: #2 -*x*+1, -*y*+1, -*z*; #5 *x*-1/2, -*y*+1/2, *z*+1/2; #6 *x*, *y*+1, *z*; #7 -*x*+3/2, *y*+1/2, -*z*+1/2.							
Complex **4**							
N(1)-Zn(1)	2.002(4)	O(4)-Zn(1)	2.067(3)	O(10)-Zn(2)	2.068(3)	O(16)-Zn(3)	1.975(4)
N(4)-Zn(4)	1.978(5)	O(5)-Zn(2)	2.039(3)	O(13)-Zn(2)	2.028(3)	Cl(1)-Zn(3)	2.232(2)
N(5)-Zn(3)	2.015(5)	O(6)-Zn(1)	2.051(3)	O(14)-Zn(1)	2.038(3)	Zn(1)-Zn(2)	3.0466(8)
N(7)-Zn(2)	2.005(4)	O(9)-Zn(1)	2.073(3)	O(15)-Zn(4)	1.927(4)	Zn(3)-O(2)$^{\#5}$	1.967(4)
O(3)-Zn(2)	2.038(3)	Zn(4)-O(8)$^{\#4}$	1.934(5)	Zn(4)-O(1)$^{\#5}$	1.980(4)	N(1)-Zn(1)-O(14)	105.64(14)
N(1)-Zn(1)-O(6)	95.18(15)	N(7)-Zn(2)-O(13)	97.84(14)	O(3)-Zn(2)-O(10)	85.69(14)	O(15)-Zn(4)-O(8)$^{\#4}$	101.18(19)
O(14)-Zn(1)-O(6)	92.01(14)	N(7)-Zn(2)-O(3)	99.72(14)	O(5)-Zn(2)-O(10)	152.06(15)	O(15)-Zn(4)-N(4)	110.65(18)
N(1)-Zn(1)-O(4)	103.02(14)	O(13)-Zn(2)-O(3)	161.87(14)	O(2)$^{\#5}$-Zn(3)-O(16)	118.32(18)	O(8)$^{\#4}$-Zn(4)-N(4)	135.9(2)
O(14)-Zn(1)-O(4)	151.33(14)	N(7)-Zn(2)-O(5)	103.91(15)	O(2)$^{\#5}$-Zn(3)-N(5)	96.08(18)	O(15)-Zn(4)-O(1)$^{\#5}$	119.55(17)
O(6)-Zn(1)-O(4)	86.09(14)	O(13)-Zn(2)-O(5)	92.16(14)	O(16)-Zn(3)-N(5)	103.83(17)	O(8)$^{\#4}$-Zn(4)-O(1)$^{\#5}$	94.2(2)
N(1)-Zn(1)-O(9)	103.16(15)	O(3)-Zn(2)-O(5)	88.00(14)	O(2)$^{\#5}$-Zn(3)-Cl(1)	117.20(15)	N(4)-Zn(4)-O(1)$^{\#5}$	95.7(2)
O(14)-Zn(1)-O(9)	87.32(14)	N(7)-Zn(2)-O(10)	103.97(16)	O(16)-Zn(3)-Cl(1)	107.53(13)	O(4)-Zn(1)-O(9)	85.52(13)
O(6)-Zn(1)-O(9)	161.14(15)	O(13)-Zn(2)-O(10)	85.72(14)	N(5)-Zn(3)-Cl(1)	112.58(16)		
Symmetry code: #4 -*x*+1, -*y*+2, -*z*; #5 *x*-1/2, -*y*+3/2, *z*-1/2.							
Complex **5**							
Cd(1)-N(3)	2.212(13)	Cd(1)-O(5)	2.306(10)	Cd(2)-O(3)$^{\#5}$	2.256(10)	Cd(2)-O(2)	2.297(10)
Cd(1)-O(8)$^{\#3}$	2.249(10)	Cd(1)-O(4)$^{\#4}$	2.324(10)	Cd(2)-O(7)$^{\#6}$	2.261(10)	Cd(2)-O(5)	2.333(9)
Cd(1)-O(1)	2.272(10)	Cd(1)-O(6)	2.462(10)	Cd(2)-N(1)	2.269(12)	N(3)-Cd(1)-O(8)$^{\#3}$	98.9(4)
N(3)-Cd(1)-O(1)	88.5(4)	O(5)-Cd(1)-O(4)$^{\#4}$	87.8(4)	O(8)$^{\#3}$-Cd(1)-O(4)$^{\#4}$	86.0(4)	O(3)$^{\#5}$-Cd(2)-O(2)	91.7(4)
O(8)$^{\#3}$-Cd(1)-O(1)	97.2(4)	N(3)-Cd(1)-O(6)	85.5(4)	O(1)-Cd(1)-O(4)$^{\#4}$	176.7(4)	O(7)$^{\#6}$-Cd(2)-O(2)	168.7(4)
N(3)-Cd(1)-O(5)	139.9(4)	O(8)$^{\#3}$-Cd(1)-O(6)	174.5(4)	O(3)$^{\#5}$-Cd(2)-O(7)$^{\#6}$	98.5(4)	N(1)-Cd(2)-O(2)	99.2(4)
O(8)$^{\#3}$-Cd(1)-O(5)	120.9(4)	O(1)-Cd(1)-O(6)	86.2(3)	O(3)$^{\#5}$-Cd(2)-N(1)	88.2(4)	O(3)$^{\#5}$-Cd(2)-O(5)	164.0(4)
O(1)-Cd(1)-O(5)	90.8(3)	O(5)-Cd(1)-O(6)	54.5(3)	O(7)$^{\#6}$-Cd(2)-N(1)	85.9(4)	O(7)$^{\#6}$-Cd(2)-O(5)	92.1(4)
N(3)-Cd(1)-O(4)$^{\#4}$	90.6(4)	O(4)$^{\#4}$-Cd(1)-O(6)	90.6(4)	O(2)-Cd(2)-O(5)	76.9(4)	N(1)-Cd(2)-O(5)	104.5(4)
Symmetry codes: #3 *x*, *y*, *z*+1; #4 *x*+1, *y*, *z*; #5 -*x*, -*y*, -*z*+1; #6 -*x*+1, -*y*, -*z*.							
Complex **6**							
Cd(1)-O(3)$^{\#1}$	2.238(6)	Cd(1)-O(2)	2.319(6)	Cd(2)-N(4)$^{\#3}$	2.248(5)	Cd(2)-O(1)	2.349(6)
Cd(1)-O(7)$^{\#2}$	2.238(5)	Cd(1)-O(5)	2.321(5)	Cd(2)-O(8)$^{\#4}$	2.288(5)	Cd(2)-O(2)	2.577(6)
Cd(1)-N(1)	2.260(6)	Cd(2)-O(6)	2.230(5)	Cd(2)-O(4)$^{\#5}$	2.288(6)	O(3)$^{\#1}$-Cd(1)-O(7)$^{\#2}$	102.0(2)
O(3)$^{\#1}$-Cd(1)-N(1)	85.9(2)	O(7)$^{\#2}$-Cd(1)-O(5)	89.0(2)	O(6)-Cd(2)-O(4)$^{\#5}$	87.9(2)	O(4)$^{\#5}$-Cd(2)-O(1)	174.5(2)
O(7)$^{\#2}$-Cd(1)-N(1)	91.6(2)	N(1)-Cd(1)-O(5)	105.93(19)	N(4)$^{\#3}$-Cd(2)-O(4)$^{\#5}$	91.2(2)	O(6)-Cd(2)-O(2)	85.62(18)
O(3)$^{\#1}$-Cd(1)-O(2)	90.2(2)	O(2)-Cd(1)-O(5)	76.4(2)	O(8)$^{\#4}$-Cd(2)-O(4)$^{\#5}$	88.4(2)	N(4)$^{\#3}$-Cd(2)-O(2)	144.98(19)
O(7)$^{\#2}$-Cd(1)-O(2)	161.6(2)	O(6)-Cd(2)-N(4)$^{\#3}$	93.7(2)	O(6)-Cd(2)-O(1)	93.9(2)	O(8)$^{\#4}$-Cd(2)-O(2)	93.7(2)
N(1)-Cd(1)-O(2)	103.08(19)	O(6)-Cd(2)-O(8)$^{\#4}$	175.0(2)	N(4)$^{\#3}$-Cd(2)-O(1)	93.9(2)	O(4)$^{\#5}$-Cd(2)-O(2)	123.7(2)
O(3)$^{\#1}$-Cd(1)-O(5)	163.7(2)	N(4)$^{\#3}$-Cd(2)-O(8)$^{\#4}$	89.7(2)	O(8)$^{\#4}$-Cd(2)-O(1)	89.5(2)	O(1)-Cd(2)-O(2)	51.4(2)
Symmetry codes: #1 -*x*+1, -*y*, -*z*+1; #2 -*x*, -*y*, -*z*+2; #3 *x*+1, -*y*+1/2, *z*+1/2; #4 *x*+1, *y*, *z*; #5 *x*, *y*, *z*+1.							