Supporting Information for the Manuscript:

Novel Coordination Polymers of Zn(II) and Cd(II) Tuned by different Aromatic Polycarboxylates: Synthesis, Structures and Photocatalytic Properties

Ming Li, Lu Liu, Lin Zhang, Xiaofeng Lv, Jie Ding*, Hongwei Hou*, Yaoting Fan

^aThe College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou 450052, P. R. China

Author for correspondence: Prof. Jie Ding, E-mail: jieding@zzu.edu.cn

Prof. Hongwei Hou, E-mail: houhongw@zzu.edu.cn

Complex	1	2	3	4	5	6
Formula	$C_{27}H_{24}CdN_4O_4$	$C_{56}H_{58}Zn_3N_8O_{18}$	$C_{75}H_{74}Cd_3N_6O_{16}$	$C_{28}H_{26}Zn_{2}N_{4}O_{8}$	$C_{24}H_{21}CdN_4O_4\\$	$C_{33}H_{32}CdN_4O_8S$
fw	580.90	1327.21	1736.66	677.27	541.85	757.09
T/K	293(2)	293(2)	293(2)	293(2)	293(2)	293(2)
λ (Mo K), Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Cryst syst	Monoclinic	Triclinic	Triclinic	Monoclinic	Triclinic	Monoclinic
Space group	P2(1)/c	P-1	P-1	P2(1)/c	P-1	P2(1)/c
a (Å)	12.761(3)	9.4806(19)	12.156(2)	11.650(2)	9.4698(19)	12.0052(2)
b (Å)	14.961(3)	18.127(4)	18.590(4)	15.490(3)	11.079(2)	18.834(4)
c (Å)	17.532(3)	18.693(4)	21.024(4)	17.108(6)	11.161(2)	16.723(6)
α(°)	90	61.88(3)	74.05(3)	90	77.45(3)	90
β(°)	132.259(19)	83.98(3)	75.94(3)	115.37(2)	78.01(3)	123.27
γ(°)	90	86.35(3)	75.58(3)	90	85.11(3)	90
V (Å ³)	2477.3(11)	2817.3(10)	4345.8(14)	2789.5(12)	1117.1(4)	3161.4(14)
Ζ	4	2	2	4	2	4
$D_{\text{calcd}}(\mathbf{g}\cdot\mathbf{cm}^{-3})$	1.558	1.565	1.263	1.613	1.611	1.591
abs coeff (mm ⁻¹)	0.923	1.349	0.786	1.778	1.017	0.816
<i>F</i> (000)	1176	1368	1676	1384	546	1544
θ (°)	2.08-28.05	2.15-25.50	1.36-25.50	1.86-25.49	1.88-27.91	2.03-25.50
R(int)	0.0357	0.0528	0.0970	0.0778	0.0553	0.0278
GOF	1.002	1.032	0.999	1.050	0.959	0.999
R_I (I>2sigma(I)) ^a	0.0411	0.0643	0.0685	0.0824	0.0567	0.0419
wR ₂ (I>2sigma(I)) ^b	0.1337	0.1983	0.1950	0.3068	0.1407	0.1658

Table S1. Crystallographic data and structure refinement details for complex 1-6^{a,b}

 ${}^{a}R_{1} = \sum ||F_{o}| - |F_{c}|| \sum / |F_{o}| \cdot {}^{b}wR_{2} = [\sum w(F_{o}^{2} - F_{c}^{2})^{2} / \sum w(F_{o}^{2})^{2}]^{1/2}.$

	Compound 1					
	Cd(1)-O(3)#1	2.278(3)	O(3)#1-Cd(1)-O(1)	152.52(11)		
Cdil)Atil)2.92(3)N(1-Q(1)(0))1.94(1)Cdil)O(1)2.34(3)(X)(1-Q(1)-Q)1.92(1)Cdil)O(2)2.44(3)(X)(1-Q(1)-Q)5.1(8)Cdil)O(1)2.27(3)(X)(1-Q(1)-Q)5.1(8)O(3-C(1)P32.45(3)(X)(1-Q(1)-Q)5.1(8)O(3-C(1)P32.45(3)(X)(1-Q(1)-Q)5.1(8)O(3-C(1)P32.45(3)(X)(1-Q(1)-Q)5.1(8)O(3+C(1)N(1)8.92(1)(X)(1-Q(1)-Q)10.28(1)O(3+C(1)N(1)8.92(1)(X)(1-Q(1)-Q)10.28(1)O(3+C(1)N(1)8.92(1)(X)(1-Q(1)-Q)10.28(1)O(3+C(1)N(1)8.92(1)(X)(1-Q(1)-Q)10.28(1)O(3+C(1)N(1)19.3(3)(X)(1-Q(1)-Q)10.3(1)N(1)P2(1)19.3(3)(X)(1-Q(1)-Q)10.3(1)O(3+C(1)N(1)19.3(3)(X)(1-Q(1)-Q)10.3(1)T(1)P3(1)19.3(3)(Q)2(1)O(3)10.3(1)Z(1)O(1)19.3(3)(Q)2(1)O(3)10.3(1)Z(1)O(2)19.3(1)(Q)2(1)O(3)10.3(1)Z(1)O(3)19.3(1)(Q)2(1)O(3)10.3(1)Z(1)O(3)19.3(1)(Q)2(1)O(3)10.3(1)Z(1)O(3)19.3(1)(Q)2(1)O(3)11.6(1)Z(1)O(3)19.4(1)(Q)2(1)O(3)11.6(1)Z(2)O(3)19.4(1)(Q)2(1)O(3)11.6(1)Z(2)O(3)19.4(1)(Q)2(1)O(3)11.6(1)Z(1)O(3)19.4(1)(Q)2(1)O(3)11.6(1)Z(1)O(3)19.4(1)(Q)2(1)O(3)11.6(1)Z(1)O(3) <td>Cd(1)-N(4)#2</td> <td>2.287(3)</td> <td>N(4)#2-Cd(1)-O(1)</td> <td>93.24(10)</td>	Cd(1)-N(4)#2	2.287(3)	N(4)#2-Cd(1)-O(1)	93.24(10)		
Cdi()-0(1)2340(3)O(3)=Cd(1)-0(2)1.6.3.5(9)Cd()-0(2)2446(2)N()-Cd(1)-0(2)9.5.16(8)O(3)-Cd(1)-0(2)25.16(8)S0.00O(3)-Cd(1)-O(4)25.00(8)S0.00O(3)-Cd(1)-O(4)25.00(8)S0.00O(3)-Cd(1)-O(4)25.00(8)S0.00(8)O(3)-Cd(1)-O(4)25.00(8)N(3)-Cd(1)-O(4)25.00(8)O(3)-Cd(1)-O(4)01-O(1)-O(4)10.52(1)-O(1)O(3)-Cd(1)-O(4)10.30(1)O(1)-Cd(1)-O(4)10.52(1)-O(1)O(3)-Cd(1)-O(4)10.30(1)O(1)-Cd(1)-O(4)10.52(1)-O(1)O(3)-Cd(1)-O(4)10.30(1)O(1)-Cd(1)-O(4)10.52(1)-O(1)Nymetry case-st = +1 + - + + + + + + + + + + + + + + + +	Cd(1)-N(1)	2.292(3)	N(1)-Cd(1)-O(1)	104.94(11)		
Cd(I)O(2)2446(2)N(4)92-Cd(I)O(2)1453(9)Cd(I)O(4)PI245(3)O(I)Cd(I)O(2)55.16(8)O(3)Cd(I)P3227(3)O(I)Cd(I)O(4)(1)55.009)O(3)Cd(I)P32287(3)N(I)Cd(I)O(4)(1)95.87(9)O(3)Cd(I)P32287(3)N(I)Cd(I)O(4)(1)1052(1)O(3)Cd(I)P30130(1)N(I)Cd(I)O(4)(1)1052(1)O(3)FLC(I)N(1)1093(1)O(I)Cd(I)O(4)(1)1052(1)O(3)FLC(I)N(1)1093(1)O(I)Cd(I)O(4)(1)1053(1)N(I)C(I)N(1)1093(1)O(I)Cd(I)O(4)(1)1053(1)N(I)C(I)N(1)1093(1)O(I)Cd(I)O(4)(1)1053(1)Zd(I)O(1)1953(1)O(I)C2(I)O(5)(1)1053(1)Zd(I)O(2)1963(1)O(I)C2(I)O(5)(1)11274(1)Zd(I)O(2)1993(1)O(I)C2(I)O(5)(1)1070(1)Zd(I)O(2)1993(1)O(I)C2(I)O(3)(1)1070(1)Zd(I)O(1)1993(1)O(I)C2(I)O(1)1070(1)Zd(I)O(1)1993(1)O(I)C2(I)O(1)1037(1)Zd(I)O(1)1993(1)O(I)C2(I)O(1)1133(1)Zd(I)O(1)1993(1)O(I)C2(I)O(1)1133(1)Zd(I)O(1)1993(1)O(I)C2(I)O(1)1133(1)Zd(I)O(1)1993(1)O(I)C2(I)O(1)1133(1)Zd(I)O(1)1993(1)O(I)C2(I)O(1)1133(1)Zd(I)O(1)1993(1)O(I)C2(I)O(1)1133(1)Zd(I)O(1)1993(1)O(I)C2(I)O(1)1133(1)Zd(I)O(1)1993(1)O(I)C2(I)O(1)1133(1)Zd(I)O(1)19	Cd(1)-O(1)	2.304(3)	O(3)#1-Cd(1)-O(2)	101.24(10)		
Cd(I)O(J)FI249(3)N(I)-Cd(I)-O(2)95.1(9)O(3)-Cd(I)F3247(3)O(3)-Cd(I)-O(3)-I55.0(9)O(3)-Cd(I)F32287(3)N(4)2-Cd(I)-O(4)F110.52(1)O(3)-Cd(I)-N(4)F210.30(1)N(I)-Cd(I)-O(4)F110.52(1)O(3)-I-Cd(I)-N(4)F110.32(1)0(2)-Cd(I)-O(4)F110.28(1)OO(3)-I-Cd(I)-N(4)F110.32(1)0(2)-Cd(I)-O(4)F110.28(1)ON(4)-2Cd(I)-N(1)10.93(3)O(2)-Cd(I)-O(4)F110.28(1)ON(4)-2Cd(I)-N(1)10.93(3)O(2)-Cd(I)-O(4)F110.28(1)ON(4)-2Cd(I)-N(1)10.93(3)O(2)-Cd(I)-O(4)F110.28(1)ON(4)-2Cd(I)-N(1)10.93(3)O(2)-Cd(I)-O(3)F111.5(1)OZd(I)-O(2)1.96(3)O(4)-Zd(I)-O(5)F111.27(1)SZd(I)-O(3)1.99(4)O(1)-Zd(I)-N(4)11.27(1)SZd(I)-O(3)1.99(4)O(2)-Zd(I)-N(4)11.03(1)CZd(2)-O(3)1.99(4)O(5)-Zd(I)-N(4)11.03(1)CZd(2)-O(1)-I11.99(4)O(5)-Zd(I)-N(4)11.61(3)Zd(2)-O(1)-I11.99(4)O(9)-Zd(2)-O(1)-I111.61(3)Zd(2)-O(1)-I11.99(4)O(9)-Zd(2)-N(1)-I111.61(3)Zd(2)-O(1)-I11.99(4)O(9)-Zd(2)-N(1)-I111.61(3)Zd(2)-O(1)-I11.99(4)O(9)-Zd(2)-N(1)-I111.61(3)Zd(2)-O(1)-I11.99(4)O(9)-Zd(2)-N(1)-I111.61(3)Zd(2)-O(1)-I11.99(4)O(9)-Zd(2)-N(1)-I111.61(3)Zd(2)-O(1)-I11.99(4)O(9)-Zd(2)-N(1)-I111.61(3)Zd(2)-O(1)-I11.	Cd(1)-O(2)	2.446(2)	N(4)#2-Cd(1)-O(2)	145.35(9)		
0(3)-G(1)/F32,27(3)0(1)-G(1)-O(2)55.1680(4)-C(1)/F32,48(3)0(3)-I-C(1)-O(4)/F155.00(9)N(4)-C(1)/F410,43(1)N(1)-C(1)-O(4)/F110,28(1)0(3)F1-C(1)/N(1)10,83(1)0(1)-C(1)-O(4)/F110,28(1)N(4)-2C(1)-N(1)10,83(2)0(2)-C(1)-O(4)/F110,28(1)N(4)-2C(1)-N(1)10,83(2)0(2)-C(1)-O(4)/F110,28(1)N(4)-2C(1)-N(1)10,83(2)0(2)-C(1)-O(4)/F110,28(1)N(4)-2C(1)-N(1)10,83(2)0(2)-C(1)-O(4)/F110,28(1)X(1)-O(2)12,24(2)-X(2)-X(2)-X(2)-X(2)-X(2)-X(2)-X(2)-X	Cd(1)-O(4)#1	2.459(3)	N(1)-Cd(1)-O(2)	93.51(9)		
0(4)-Cd(1)#32,459(3)0(3)#1-Cd(1)-O(4)#155,009()N(4)-Cd(1)#42,287(3)N(4)/2-Cd(1)-O(4)#1446,52(0)O(3)#1-Cd(1)+N(4)#219,80(1)O(1)-Cd(1)-O(4)#180,30(8)O(3)#1-Cd(1)+N(4)19,80(1)O(1)-Cd(1)-O(4)#180,30(8)N(4)#2-Cd(1)+N(1)19,80(1)O(1)-Cd(1)-O(4)#180,30(8)N(4)#2-Cd(1)+N(1)19,80(1)O(1)-Cd(1)-O(4)#180,30(8)Symmetry code: #1 = x+1, x-1 + 2 + 2 + 2 + x + x+1, x-1 + 2 + 2 + 2 + x + x+1, x-1 + 2 + 2 + x + x+1, x+1 + x + x + x+1 + x + x+1 + x + x+1 + x + x	O(3)-Cd(1)#3	2.277(3)	O(1)-Cd(1)-O(2)	55.16(8)		
N(A)-G(I)%42,287(3)N(A)2C(I)-O(A)%19,587(9)O(3)F1-C(I),N(M)?2103 0(1)(1)-C(I)-O(A)%1102 587(1)O(3)F1-C(I),N(N)103 0(3)(1)-C(I)-O(A)%1102 587(1)N(M)-C(I),N(N)103 0(3)(1)-C(I)-O(A)%1102 587(1)Symmetry-cotes:#1=x+1;z+z=x+z+z+z+z+z+z+z+z+z+z+z+z+z+z+z+z+z+	O(4)-Cd(1)#3	2.459(3)	O(3)#1-Cd(1)-O(4)#1	55.00(9)		
<table-container><math> <table-cell>0(3)#1-Cd(1)-N(4)#2104.30(1)N(1)-Cd(1)-O(4)#1104.32(1)0(3)#1-Cd(1)-N(1)89.92(1)O(1)-Cd(1)-O(4)#1102.89(1)N(4)#2-Cd(1)-N(1)108.89(0)O(2)-Cd(1)-O(4)#180.3(8)Symmety-code::#1 = x+1, y-x1/2: x2 = x, y-y1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2 = x, y-y1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2 = x, y-y1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2 = x, y-y1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2 = x, y-y1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2 = x, y-y1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2 = x-y-y1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2 = x-y-y1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2 = x-y-y1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2 = x-y-y1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2x-y-y1/2; x21:x2#4 = xy = 1/2; x21:x2x4,x4x4,x4#4 = x1 = xy = 1/2; x21:x2x4,x4x4,x4#4 = x1 = x4; x21:x4x4,x4x4,x4#4 = x4 = x4; x4; x4x</table-cell></math></table-container>	N(4)-Cd(1)#4	2.287(3)	N(4)#2-Cd(1)-O(4)#1	95.87(9)		
<table-container><math><table-row>0(3)41-Cd(1)-N(1)89.0(1)0(1)-Cd(1)-O(4)fl102.8(0)N(4)2-Cd(1)-N(1)108.3(3)0(2)-Cd(1)-O(4)fl80.3(3)Symmetry codes: #1 = x1, y2 + 2/2, x1 + 2/2, x1</table-row></math></table-container>	O(3)#1-Cd(1)-N(4)#2	104.30(11)	N(1)-Cd(1)-O(4)#1	140.52(10)		
<table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-container><table-row><table-row><table-row><table-row><table-container><table-container><table-container></table-container></table-container></table-container></table-row><table-row><table-row><table-row><table-container><table-container></table-container></table-container></table-row><table-row><table-row><table-row><table-container><table-container></table-container></table-container></table-row><table-row><table-row><table-row><table-container><table-container></table-container></table-container></table-row><table-row><table-row><table-row><table-container></table-container></table-row><table-row></table-row><table-row></table-row><table-row><table-container><table-container></table-container></table-container></table-row><table-row><table-row><table-row><table-container><table-container></table-container></table-container></table-row><table-row><table-row><table-row><table-container></table-container></table-row><table-row></table-row><table-row></table-row><table-row></table-row><table-row></table-row><table-row></table-row><table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-row></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container></table-container>	O(3)#1-Cd(1)-N(1)	89.02(11)	O(1)-Cd(1)-O(4)#1	102.89(10)		
Symmetry codes: #1 = x+1, y-1/2, z+1/2; #2 = x, y+1/2, z+1/2; #4 = x, y+1/2, z+1/2; #4 = x, y+1/2, z+1/2; Compound Zn(1)-O(4) 192(3) 0(4)-Zn(1)-O(5)#1 97.08(16) Zn(1)-O(5)#1 1993(4) O(12)-Zn(1)-O(5)#1 12.74(15) Zn(1)-O(5)#1 1993(4) O(12)-Zn(1)-O(5)#1 12.74(15) Zn(1)-O(5)#1 1993(4) O(12)-Zn(1)-N(4) 10.70(16) Zn(2)-O(6) 1934(3) O(12)-Zn(1)-N(4) 10.70(16) Zn(2)-O(9)#2 1967(4) O(5)#1-Zn(1)-N(4) 10.70(16) Zn(2)-O(9)#2 1967(4) O(5)Zn(2)-O(9)#2 116.67(17) Zn(2)-O(1)#1 1991(4) O(6)-Zn(2)-O(1)#1 11.03(17) Zn(2)-O(1)#1 1991(4) O(6)-Zn(2)-O(1)#1 11.03(17) Zn(3)-O(7)#3 1997(4) O(9)#2-Zn(2)-N(5) 11.16(18) Zn(3)-N(1)#4 1997(4) O(9)#2-Zn(2)-N(5) 11.16(18) Zn(3)-N(1)#4 1997(4) O(1)-Zn(3)-N(3)#4 11.56(16) O(5)-Zn(1)#1 1993(4) O(1)-Zn(3)-N(3)#4 11.56(16) O(7)-Zn(3)#3 1994(4) O(1)-Zn(3)-N(3)#5 10.93(16) O(7)-Zn(3)#	N(4)#2-Cd(1)-N(1)	109.83(9)	O(2)-Cd(1)-O(4)#1	80.03(8)		
Here:24 = x, y+1/2, z+1/2.Lore:2n(1)-O(4)1928(3)0(4)-Zn(1)-O(2)108.85(n)Zn(1)-O(2)196(3)0(4)-Zn(1)-O(5)FI9.708(n)Zn(1)-O(5)FI1939(4)0(4)-Zn(1)-O(5)FI12.274(17)Zn(1)-O(4)1939(4)0(4)-Zn(1)-N(4)10.70(n)Zn(2)-O(9)F2196(7)0(5)FI-Zn(1)-N(4)10.70(n)Zn(2)-O(1)JFI1991(4)0(6)-Zn(2)-O(9)F216.67(17)Zn(2)-O(1)JFI1991(4)0(6)-Zn(2)-O(1)JFI11.03(17)Zn(3)-O(1)1991(4)0(6)-Zn(2)-O(1)JFI11.03(17)Zn(3)-O(7)JF31991(4)0(9)F2-Zn(2)-O(1)JFI19.87(17)Zn(3)-O(7)JF31991(4)0(9)F2-Zn(2)-O(1)JFI11.61(8)Zn(3)-O(7)JF31991(4)0(9)F2-Zn(2)-N(5)11.16(18)Zn(3)-O(7)JF31991(4)0(1)-Zn(2)-N(5)11.61(8)Zn(3)-O(7)JF31993(4)0(1)-Zn(2)-N(5)11.61(8)Zn(3)-O(7)JF31993(4)0(1)-Zn(3)-N(3)FI11.56(16)Zn(3)-O(7)JF31993(4)0(1)-Zn(3)-N(3)FI11.56(16)Qn(2)-Zn(2)F6199(1)0(1)-Zn(3)-N(3)FI11.56(16)Qn(2)-Zn(2)F6199(1)0(1)-Zn(3)-N(3)FI11.56(16)Qn(2)-Zn(2)F6199(1)0(1)-Zn(3)-N(3)FI11.56(16)Qn(2)-Zn(2)F6199(1)0(1)-Zn(3)-N(3)FI11.56(16)Qn(2)-Zn(2)F6199(1)0(1)-Zn(3)-N(3)FI11.92(16)Qn(2)-Zn(2)F6199(1)0(1)-Zn(3)-N(3)FI11.92(16)Qn(2)-Zn(2)F6199(1)	Symmetry codes: $\#1 = x+1, -y-1/2, z$	x+1/2; #2 = x, -y+1/2, z-1/2; #3 = x	-1, -y-1/2, z-1/2;			
Image: Control Za(1)-O(1) 1928(3) O(4)-Za(1)-O(12) 108.85(n) Za(1)-O(12) 196(3) O(4)-Za(1)-O(5)#1 12.74(5) Za(1)-O(5)#1 199(4) O(4)-Za(1)-O(5)#1 12.74(5) Za(1)-O(5)#1 199(4) O(4)-Za(1)-N(4) 12.74(7) Za(2)-O(6) 1934(3) O(2)-Za(1)-N(4) 103.70(7) Za(2)-O(1)#1 199(4) O(5)#1-Za(1)-N(4) 103.70(7) Za(2)-O(1)#1 199(4) O(6)-Za(2)-O(9)#2 16.67(7) Za(2)-O(1)#1 199(4) O(6)-Za(2)-O(1)#1 11.03(7) Za(3)-O(1)#1 199(3) O(6)-Za(2)-N(5) 11.85(7) Za(3)-O(1)#3 199(4) O(9)-Za(2)-N(5) 11.86(8) Za(3)-N(3)#3 199(3) O(1)-Za(3)-N(3)# 11.86(1) Za(3)-N(3)#3 199(3) O(1)-Za(3)-N(3)# 10.93(1) O(3)-Za(1)#1 199(4) O(1)-Za(3)-N(3)# 11.36(1) O(3)-Za(1)#1 199(4) O(1)-Za(3)-N(3)# 11.37(1)G) O(1)-Za(3)#3 199(4) O(1)-Za(3)-N(3)# 11.37(1)G)	#4 = x, -y+1/2, z+1/2.					
		Com	pound 2			
Zn(1)-O(12) 1966(3) O(4)-Zn(1)-O(5)#1 97.08(16) Zn(1)-O(5)#1 1.93(3) O(12)-Zn(1)-O(5)#1 112.74(15) Zn(1)-N(4) 1.93(3) O(12)-Zn(1)-N(4) 10.70(16) Zn(2)-O(6)#2 1.967(4) O(5)#1-Zn(1)-N(4) 10.70(16) Zn(2)-O(1)#1 1.91(4) O(6)-Zn(2)-O(9)#2 16.67(17) Zn(2)-O(1)#1 1.91(3) O(6)-Zn(2)-O(1)#1 11.03(17) Zn(3)-O(1) 1.92(4) O(9)#2-Zn(2)-O(1)#1 9.07(16) Zn(3)-O(1)#3 1.940(4) O(6)-Zn(2)-N(5) 11.6(18) Zn(3)-O(1)#4 1.997(4) O(9)#2-Zn(2)-N(5) 11.6(18) Zn(3)-N(1)#4 1.997(4) O(1)#1-Zn(2)-N(5) 10.84(18) O(5)-Zn(1)#1 1.993(4) O(1)-Zn(3)-N(1)#4 11.5(16) O(7)-Zn(3)#3 1.994(4) O(1)-Zn(3)-N(1)#4 11.5(16) O(1)-Zn(2)#1 1.991(4) O(1)-Zn(3)-N(1)#4 11.5(16) O(1)-Zn(2)#1 1.991(4) O(1)-Zn(3)-N(1)#4 13.08(16) N(1)-Zn(2)#1 1.991(4) O(1)-Zn(3)-N(1)#5 13.08(16) <	Zn(1)-O(4)	1.928(3)	O(4)-Zn(1)-O(12)	108.85(16)		
Zn(1)-0(5)#1 193(4) 0(12)-Zn(1)-0(5)#1 112.74(15) Zn(1)-N(4) 1.997(4) 0(4)-Zn(1)-N(4) 122.74(17) Zn(2)-0(6) 1.93(3) 0(12)-Zn(1)-N(4) 10.70(16) Zn(2)-0(9)#2 1.967(4) 0(5)#1-Zn(1)-N(4) 10.37(17) Zn(2)-0(1)#1 1.919(4) 0(6)-Zn(2)-0(1)#1 11.03(17) Zn(2)-N(5) 1.93(4) 0(9)#2-Zn(2)-0(1)#1 90.7(16) Zn(3)-O(1)#3 1.940(4) 0(6)-Zn(2)-N(5) 11.85(17) Zn(3)-N(1)#4 1.997(4) 0(9)#2-Zn(2)-N(5) 11.85(17) Zn(3)-N(1)#4 1.997(4) 0(1)#1-Zn(2)-N(5) 10.84(18) O(5)-Zn(1)#1 1.993(4) 0(1)-Zn(3)-N(1)#4 11.5(16) O(7)-Zn(3)#3 1.940(4) 0(1)-Zn(3)-N(1)#4 11.5(16) O(9)-Zn(2)#6 1.991(4) 0(1)-Zn(3)-N(1)#4 11.5(16) O(1)-Zn(3)#3 1.991(4) 0(1)-Zn(3)-N(1)#4 11.3(1(6) O(1)-Zn(3)#1 1.991(4) 0(1)-Zn(3)-N(1)#5 11.30(16) N(1)-Zn(3)#7 1.991(4) 0(1)-Zn(3)-N(3)#5 10.94(16)	Zn(1)-O(12)	1.966(3)	O(4)-Zn(1)-O(5)#1	97.08(16)		
Zn(1)-N(4) 1997(4) O(4)-Zn(1)-N(4) 122.74(17) Zn(2)-O(6) 1934(3) O(12)-Zn(1)-N(4) 100.70(6) Zn(2)-O(9)#2 1967(4) O(5)#1-Zn(1)-N(4) 103.79(17) Zn(2)-O(1)#1 1991(4) O(6)-Zn(2)-O(9)#2 116.67(17) Zn(2)-N(5) 1.993(4) O(6)-Zn(2)-O(1)#1 111.03(17) Zn(3)-O(1)#1 1.929(4) O(9)#2-Zn(2)-O(1)#1 90.71(6) Zn(3)-O(7)#3 1.940(4) O(9)#2-Zn(2)-N(5) 118.57(17) Zn(3)-N(1)#4 1.997(4) O(9)#2-Zn(2)-N(5) 1048(18) O(5)-Zn(1)#1 1.991(4) O(1)-Zn(2)-N(5) 1048(18) O(5)-Zn(1)#1 1.991(4) O(1)-Zn(3)-N(1)#4 111.56(16) O(7)-Zn(3)#3 1.994(4) O(1)-Zn(3)-N(1)#4 113.71(16) O(1)-Zn(3)#1 1.991(4) O(1)-Zn(3)-N(1)#4 113.71(16) O(1)-Zn(3)#3 1.991(4) O(1)-Zn(3)-N(8)#5 113.08(16) N(1)-Zn(3)#7 1.997(4) O(7)#3-Zn(3)-N(8)#5 13.08(16) N(1)-Zn(3)#7 1.997(4) O(1)-Zn(3)-N(8)#5 13.98(16)	Zn(1)-O(5)#1	1.993(4)	O(12)-Zn(1)-O(5)#1	112.74(15)		
Zn(2)-O(6) 1934(3) O(12)-Zn(1)-N(4) 110.70(16) Zn(2)-O(9)#2 1.967(4) O(5)#1-Zn(1)-N(4) 103.79(17) Zn(2)-O(1)#1 1.991(4) O(6)-Zn(2)-O(9)#2 116.67(17) Zn(2)-O(1)#1 1.993(4) O(6)-Zn(2)-O(1)#1 111.03(17) Zn(3)-O(1) 1.992(4) O(9)#2-Zn(2)-O(1)#1 90.17(6) Zn(3)-O(7)#3 1.940(4) O(6)-Zn(2)-N(5) 118.57(17) Zn(3)-N(1)#4 1.997(4) O(9)#2-Zn(2)-N(5) 111.6(18) Zn(3)-N(1)#4 1.997(4) O(1)/Zn(2)-N(5) 104.86(18) O(5)-Zn(1)#1 1.993(4) O(1)-Zn(2)-N(5) 104.86(18) O(5)-Zn(1)#1 1.993(4) O(1)-Zn(3)-N(1)#4 111.56(16) O(7)-Zn(3)#3 1.994(4) O(1)-Zn(3)-N(1)#4 113.71(16) O(1)-Zn(2)#1 1.991(4) O(1)-Zn(3)-N(8)#5 113.88(16) N(1)-Zn(3)#7 1.997(4) O(1)#2-Zn(3)-N(8)#5 113.08(16) N(1)-Zn(3)#7 0.997(4) N(1)#4-Zn(3)-N(8)#5 104.91(18) Symmetry codes: #1 = -x+1, -y+2 + : x = x, y x +1; #3 = -x+1, -y+1, -y x = +x + y, -y, z = x + y + y	Zn(1)-N(4)	1.997(4)	O(4)-Zn(1)-N(4)	122.74(17)		
Zn(2)-O(9)#2 1967(4) O(5)#1-Zn(1)-N(4) 103.79(17) Zn(2)-O(11)#1 1.991(4) O(6)-Zn(2)-O(9)#2 116.67(17) Zn(2)-N(5) 1.993(4) O(6)-Zn(2)-O(11)#1 111.03(17) Zn(3)-O(1) 1.929(4) O(9)#2-Zn(2)-O(11)#1 90.17(6) Zn(3)-O(7)#3 1.940(4) O(6)-Zn(2)-N(5) 118.57(17) Zn(3)-N(1)#4 1.997(4) O(9)#2-Zn(2)-N(5) 111.16(18) Zn(3)-N(8)#5 2.008(4) O(1)#1-Zn(2)-N(5) 104.86(18) O(5)-Zn(1)#1 1.997(4) O(1)-Zn(3)-O(7)#3 100.93(16) O(7)-Zn(3)#3 1.940(4) O(1)-Zn(3)-N(1)#4 11.56(16) O(9)-Zn(2)#6 1.967(4) O(1)-Zn(3)-N(1)#4 113.71(16) O(1)-Zn(2)#1 1.991(4) O(1)-Zn(3)-N(8)#5 112.93(18) N(1)-Zn(3)#7 1.997(4) O(7)#3-Zn(3)-N(8)#5 113.08(16) N(8)-Zn(3)#5 2.008(4) N(1)#4-Zn(3)-N(8)#5 149.91(18) Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = +x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x, 1, y, z E E Cd(1)-N(1)	Zn(2)-O(6)	1.934(3)	O(12)-Zn(1)-N(4)	110.70(16)		
Zn(2)-O(11)#1 1.991(4) O(6)-Zn(2)-O(9)#2 116.67(17) Zn(2)-N(5) 1.993(4) O(6)-Zn(2)-O(11)#1 111.03(17) Zn(3)-O(1) 1.929(4) O(9)#2-Zn(2)-O(11)#1 90.17(16) Zn(3)-O(7)#3 1.940(4) O(6)-Zn(2)-N(5) 118.57(17) Zn(3)-N(1)#4 1.997(4) O(9)#2-Zn(2)-N(5) 104.86(18) O(5)-Zn(1)#1 1.997(4) O(1)#1-Zn(2)-N(5) 104.86(18) O(5)-Zn(1)#1 1.993(4) O(1)-Zn(3)-O(7)#3 100.93(16) O(7)-Zn(3)#3 1.940(4) O(1)-Zn(3)-N(1)#4 111.56(16) O(7)-Zn(3)#3 1.940(4) O(7)#3-Zn(3)-N(1)#4 113.71(16) O(1)-Zn(2)#6 1.967(4) O(7)#3-Zn(3)-N(1)#4 113.71(16) O(1)-Zn(2)#1 1.991(4) O(7)#3-Zn(3)-N(8)#5 113.08(16) N(1)-Zn(3)#7 1.997(4) O(7)#3-Zn(3)-N(8)#5 113.08(16) N(8)-Zn(3)#5 2.008(4) N(1)#4-Zn(3)-N(8)#5 104.91(18) Symmetry codes: #1 = -x+1, -y+2, -x; +2 = x, y, z+1; #3 = -x+1, -y+1, -x; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z Zcd(1)-N(1) 2.265(5) O(2)-	Zn(2)-O(9)#2	1.967(4)	O(5)#1-Zn(1)-N(4)	103.79(17)		
Zn(2)-N(5) 1.993(4) 0(6)-Zn(2)-O(11)#1 11.103(17) Zn(3)-O(1) 1.929(4) 0(9)#2-Zn(2)-O(11)#1 90.17(16) Zn(3)-O(7)#3 1.940(4) 0(6)-Zn(2)-N(5) 118.57(17) Zn(3)-N(1)#4 1.997(4) 0(9)#2-Zn(2)-N(5) 111.16(18) Zn(3)-N(8)#5 2.008(4) O(1)#1-Zn(2)-N(5) 104.86(18) O(5)-Zn(1)#1 1.993(4) O(1)-Zn(3)-O(7)#3 100.93(16) O(7)-Zn(3)#3 1.940(4) O(1)-Zn(3)-N(1)#4 111.56(16) O(9)-Zn(2)#6 1.967(4) O(7)#3-Zn(3)-N(1)#4 113.71(16) O(1)-Zn(2)#1 1.991(4) O(1)-Zn(3)-N(8)#5 112.93(18) N(1)-Zn(3)#7 1.997(4) O(7)#3-Zn(3)-N(8)#5 113.08(16) N(8)-Zn(3)#5 2.008(4) N(1)#4-Zn(3)-N(8)#5 104.91(18) Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -x; #5 = -x+2, -y+1, -z; #4 = x+1, y, z, z+5 = -x+2, -y+1, -z; #7 = x-1, y, z. Y Cd(1)-N(1) 2.265(5) O(2)-Cd(1)-O(1) 55.29(17) Cd(1)-N(1) 2.265(5) O(1)-Cd(1)-O(8) 55.14(15) Cd(1)-O(7) 2.36	Zn(2)-O(11)#1	1.991(4)	O(6)-Zn(2)-O(9)#2	116.67(17)		
Zn(3)-O(1) 1.929(4) O(9)#2-Zn(2)-O(11)#1 90.17(16) Zn(3)-O(7)#3 1.940(4) O(6)-Zn(2)-N(5) 118.57(17) Zn(3)-N(1)#4 1.997(4) O(9)#2-Zn(2)-N(5) 111.16(18) Zn(3)-N(8)#5 2.008(4) O(11)#1-Zn(2)-N(5) 104.86(18) O(5)-Zn(1)#1 1.993(4) O(1)-Zn(3)-O(7)#3 100.93(16) O(7)-Zn(3)#3 1.940(4) O(1)-Zn(3)-N(1)#4 111.56(16) O(9)-Zn(2)#6 1.967(4) O(7)#3-Zn(3)-N(1)#4 113.71(16) O(1)-Zn(2)#1 1.991(4) O(1)-Zn(3)-N(8)#5 112.93(18) N(1)-Zn(3)#7 1.997(4) O(7)#3-Zn(3)-N(8)#5 113.08(16) N(8)-Zn(3)#5 2.008(4) N(1)#4-Zn(3)-N(8)#5 104.91(18) Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #7 = x-1, y, z. Te -xy, z-1; #7 = x-1, y, z. Cd(1)-N(1) 2.265(5) O(2)-Cd(1)-O(1) 55.29(17) Cd(1)-N(9) 2.276(5) N(1)-Cd(1)-O(8) 87.51(18) Cd(1)-O(7) 2.297(4) N(9)-Cd(1)-O(8) 87.51(18) Cd(1)-O(1)	Zn(2)-N(5)	1.993(4)	O(6)-Zn(2)-O(11)#1	111.03(17)		
Zn(3)-O(7)#3 1.940(4) O(6)-Zn(2)-N(5) 118.57(17) Zn(3)-N(1)#4 1.997(4) O(9)#2-Zn(2)-N(5) 111.16(18) Zn(3)-N(8)#5 2.008(4) O(1)#1-Zn(2)-N(5) 104.86(18) O(5)-Zn(1)#1 1.993(4) O(1)-Zn(3)-O(7)#3 100.93(16) O(7)-Zn(3)#3 1.940(4) O(1)-Zn(3)-N(1)#4 111.56(16) O(9)-Zn(2)#6 1.967(4) O(7)#3-Zn(3)-N(1)#4 113.71(16) O(1)-Zn(2)#1 1.991(4) O(1)-Zn(3)-N(8)#5 112.93(18) N(1)-Zn(3)#7 1.997(4) O(7)#3-Zn(3)-N(8)#5 104.91(18) Symmetry codes: #1 = -x+1, -y+2, -y = x, y, z+1; #3 = -x+1, -y+1, -y; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z. Zc4(1)-N(1) 2.265(5) O(2)-Cd(1)-O(1) 55.29(17) Cd(1)-N(1) 2.265(5) N(1)-Cd(1)-O(8) 87.51(18) Cd(1)-N(9) 2.27(4) N(9)-Cd(1)-O(8) 87.51(18) Cd(1)-O(7) 2.297(4) N(9)-Cd(1)-O(8) 87.51(18) Cd(1)-O(2) 2.36(5) O(7)-Cd(1)-O(8) 87.51(18) Cd(1)-O(2) 2.391(5) O(2)-Cd(1)-O(8) 15.98(18	Zn(3)-O(1)	1.929(4)	O(9)#2-Zn(2)-O(11)#1	90.17(16)		
Zn(3)-N(1)#4 1.997(4) O(9)#2-Zn(2)-N(5) 111.16(18) Zn(3)-N(8)#5 2.008(4) O(11)#1-Zn(2)-N(5) 104.86(18) O(5)-Zn(1)#1 1.993(4) O(1)-Zn(3)-O(7)#3 100.93(16) O(7)-Zn(3)#3 1.940(4) O(1)-Zn(3)-N(1)#4 111.56(16) O(9)-Zn(2)#6 1.967(4) O(7)#3-Zn(3)-N(1)#4 113.71(16) O(1)-Zn(2)#1 1.991(4) O(1)-Zn(3)-N(8)#5 112.93(18) N(1)-Zn(3)#7 1.997(4) O(7)#3-Zn(3)-N(8)#5 113.08(16) N(8)-Zn(3)#5 2.008(4) N(1)#4-Zn(3)-N(8)#5 104.91(18) Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z. Cd(1)-N(1) 2.265(5) O(2)-Cd(1)-O(1) 55.29(17) Cd(1)-N(1) 2.265(5) O(2)-Cd(1)-O(8) 55.19(15) 151.10(17) Cd(1)-N(9) 2.276(5) N(1)-Cd(1)-O(8) 87.51(18) 151.01(7) Cd(1)-O(7) 2.297(4) N(9)-Cd(1)-O(8) 87.51(18) 151.98(18) 151.98(18) 151.98(18) 151.98(18) 151.98(18) 15.98(18) 15.98(18)	Zn(3)-O(7)#3	1.940(4)	O(6)-Zn(2)-N(5)	118.57(17)		
Zn(3)-N(8)#52.008(4)O(11)#1-Zn(2)-N(5)104.86(18)O(5)-Zn(1)#11.993(4)O(1)-Zn(3)-O(7)#3100.93(16)O(7)-Zn(3)#31.940(4)O(1)-Zn(3)-N(1)#4111.56(16)O(9)-Zn(2)#61.967(4)O(7)#3-Zn(3)-N(1)#4113.71(16)O(11)-Zn(2)#11.991(4)O(1)-Zn(3)-N(8)#5112.93(18)N(1)-Zn(3)#71.997(4)O(7)#3-Zn(3)-N(8)#5113.08(16)N(8)-Zn(3)#52.008(4)N(1)#4-Zn(3)-N(8)#5104.91(18)Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z.Cd(1)-N(1)2.265(5)O(2)-Cd(1)-O(1)55.29(17)Cd(1)-N(9)2.276(5)N(1)-Cd(1)-O(8)151.10(17)Cd(1)-O(7)2.297(4)N(9)-Cd(1)-O(8)87.51(18)Cd(1)-O(1)2.391(5)O(2)-Cd(1)-O(8)55.14(15)Cd(1)-O(1)2.391(5)O(2)-Cd(1)-O(8)55.14(15)Cd(1)-O(8)2.424(5)O(1)-Cd(1)-O(8)94.92(18)	Zn(3)-N(1)#4	1.997(4)	O(9)#2-Zn(2)-N(5)	111.16(18)		
O(5)-Zn(1)#11.993(4)O(1)-Zn(3)-O(7)#3100.93(16)O(7)-Zn(3)#31.940(4)O(1)-Zn(3)-N(1)#4111.56(16)O(9)-Zn(2)#61.967(4)O(7)#3-Zn(3)-N(1)#4113.71(16)O(1)-Zn(2)#11.991(4)O(1)-Zn(3)-N(8)#5112.93(18)N(1)-Zn(3)#71.997(4)O(7)#3-Zn(3)-N(8)#5113.08(16)N(8)-Zn(3)#52.008(4)N(1)#4-Zn(3)-N(8)#5104.91(18)Symmetry codes: #1 = -x+1, -y+2, -y-z = x, y, z+1; #3 = -x+1, -y+1, -y-z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z.XCd(1)-N(1)2.265(5)O(2)-Cd(1)-O(1)55.29(7)Cd(1)-N(1)2.265(5)N(1)-Cd(1)-O(8)151.10(17)Cd(1)-O(7)2.297(4)N(9)-Cd(1)-O(8)87.51(18)Cd(1)-O(1)2.366(5)O(7)-Cd(1)-O(8)55.14(15)Cd(1)-O(1)2.391(5)O(2)-Cd(1)-O(8)15.98(18)Cd(1)-O(8)2.424(5)O(1)-Cd(1)-O(8)94.92(18)	Zn(3)-N(8)#5	2.008(4)	O(11)#1-Zn(2)-N(5)	104.86(18)		
O(7)-Zn(3)#31.940(4)O(1)-Zn(3)-N(1)#4111.56(16)O(9)-Zn(2)#61.967(4)O(7)#3-Zn(3)-N(1)#4113.71(16)O(11)-Zn(2)#11.991(4)O(1)-Zn(3)-N(8)#5112.93(18)N(1)-Zn(3)#71.997(4)O(7)#3-Zn(3)-N(8)#5113.08(16)N(8)-Zn(3)#52.008(4)N(1)#4-Zn(3)-N(8)#5104.91(18)Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z.Cd(1)-N(1)2.265(5)O(2)-Cd(1)-O(1)55.29(17)Cd(1)-N(1)2.265(5)N(1)-Cd(1)-O(8)151.10(17)Cd(1)-O(7)2.297(4)N(9)-Cd(1)-O(8)87.51(18)Cd(1)-O(2)2.366(5)O(7)-Cd(1)-O(8)55.14(15)Cd(1)-O(1)2.391(5)O(2)-Cd(1)-O(8)115.98(18)Cd(1)-O(8)2.42(5)O(1)-Cd(1)-O(8)94.92(18)	O(5)-Zn(1)#1	1.993(4)	O(1)-Zn(3)-O(7)#3	100.93(16)		
O(9)-Zn(2)#61.967(4)O(7)#3-Zn(3)-N(1)#4113.71(16)O(11)-Zn(2)#11.991(4)O(1)-Zn(3)-N(8)#5112.93(18)N(1)-Zn(3)#71.997(4)O(7)#3-Zn(3)-N(8)#5113.08(16)N(8)-Zn(3)#52.008(4)N(1)#4-Zn(3)-N(8)#5104.91(18)Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z.Cd(1)-N(1)2.265(5)O(2)-Cd(1)-O(1)55.29(17)Cd(1)-N(9)2.276(5)N(1)-Cd(1)-O(8)151.10(17)Cd(1)-O(7)2.297(4)N(9)-Cd(1)-O(8)87.51(18)Cd(1)-O(2)2.366(5)O(7)-Cd(1)-O(8)55.14(15)Cd(1)-O(1)2.391(5)O(2)-Cd(1)-O(8)115.98(18)Cd(1)-O(8)2.424(5)O(1)-Cd(1)-O(8)94.92(18)	O(7)-Zn(3)#3	1.940(4)	O(1)-Zn(3)-N(1)#4	111.56(16)		
O(11)-Zn(2)#11.991(4) $O(1)$ -Zn(3)-N(8)#5112.93(18)N(1)-Zn(3)#71.997(4) $O(7)$ #3-Zn(3)-N(8)#5113.08(16)N(8)-Zn(3)#52.008(4)N(1)#4-Zn(3)-N(8)#5104.91(18)Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z.Cd(1)-N(1)2.265(5) $O(2)$ -Cd(1)-O(1)55.29(17)Cd(1)-N(9)2.276(5)N(1)-Cd(1)-O(8)151.10(17)Cd(1)-O(7)2.297(4)N(9)-Cd(1)-O(8)87.51(18)Cd(1)-O(2)2.366(5) $O(7)$ -Cd(1)-O(8)55.14(15)Cd(1)-O(1)2.391(5) $O(2)$ -Cd(1)-O(8)115.98(18)Cd(1)-O(8)2.424(5) $O(1)$ -Cd(1)-O(8)94.92(18)	O(9)-Zn(2)#6	1.967(4)	O(7)#3-Zn(3)-N(1)#4	113.71(16)		
N(1)-Zn(3)#7 1.997(4) O(7)#3-Zn(3)-N(8)#5 113.08(16) N(8)-Zn(3)#5 2.008(4) N(1)#4-Zn(3)-N(8)#5 104.91(18) Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z. Columbra - x - x - x - x - x - x - x - x - x -	O(11)-Zn(2)#1	1.991(4)	O(1)-Zn(3)-N(8)#5	112.93(18)		
N(8)-Zn(3)#5 2.008(4) N(1)#4-Zn(3)-N(8)#5 104.91(18) Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z. Compound 3 Cd(1)-N(1) 2.265(5) O(2)-Cd(1)-O(1) 55.29(17) Cd(1)-N(9) 2.276(5) N(1)-Cd(1)-O(8) 151.10(17) Cd(1)-O(7) 2.297(4) N(9)-Cd(1)-O(8) 87.51(18) Cd(1)-O(2) 2.366(5) O(7)-Cd(1)-O(8) 55.14(15) Cd(1)-O(1) 2.391(5) O(2)-Cd(1)-O(8) 115.98(18) Cd(1)-O(8) 2.424(5) O(1)-Cd(1)-O(8) 94.92(18)	N(1)-Zn(3)#7	1.997(4)	O(7)#3-Zn(3)-N(8)#5	113.08(16)		
Symmetry codes: #1 = -x+1, -y+2, -z; #2 = x, y, z+1; #3 = -x+1, -y+1, -z; #4 = x+1, y, z; #5 = -x+2, -y+1, -z+1; #6 = x, y, z-1; #7 = x-1, y, z.Compound 3Cd(1)-N(1)2.265(5) $O(2)$ -Cd(1)- $O(1)$ 55.29(17)Cd(1)-N(9)2.276(5) $N(1)$ -Cd(1)- $O(8)$ 151.10(17)Cd(1)-O(7)2.297(4) $N(9)$ -Cd(1)- $O(8)$ 87.51(18)Cd(1)-O(2)2.366(5) $O(7)$ -Cd(1)- $O(8)$ 55.14(15)Cd(1)-O(1)2.391(5) $O(2)$ -Cd(1)- $O(8)$ 115.98(18)Cd(1)-O(8)2.424(5) $O(1)$ -Cd(1)- $O(8)$ 94.92(18)	N(8)-Zn(3)#5	2.008(4)	N(1)#4-Zn(3)-N(8)#5	104.91(18)		
Cd(1)-N(1)2.265(5)O(2)-Cd(1)-O(1)55.29(17)Cd(1)-N(9)2.276(5)N(1)-Cd(1)-O(8)151.10(17)Cd(1)-O(7)2.297(4)N(9)-Cd(1)-O(8)87.51(18)Cd(1)-O(2)2.366(5)O(7)-Cd(1)-O(8)55.14(15)Cd(1)-O(1)2.391(5)O(2)-Cd(1)-O(8)115.98(18)Cd(1)-O(8)2.424(5)O(1)-Cd(1)-O(8)94.92(18)	Symmetry codes: $\#1 = -x+1, -y+2, -z; \#2 = x, y, z+1; \#3 = -x+1, -y+1, -z; \#4 = x+1, y, z; \#5 = -x+2, -y+1, -z+1; \#6 = x, y, z-1; \#7 = x-1, y, z.$					
Cd(1)-N(9) 2.276(5) N(1)-Cd(1)-O(8) 151.10(17) Cd(1)-O(7) 2.297(4) N(9)-Cd(1)-O(8) 87.51(18) Cd(1)-O(2) 2.366(5) O(7)-Cd(1)-O(8) 55.14(15) Cd(1)-O(1) 2.391(5) O(2)-Cd(1)-O(8) 115.98(18) Cd(1)-O(8) 2.424(5) O(1)-Cd(1)-O(8) 94.92(18)	Cd(1)-N(1)	2 265(5)	0(2)-Cd(1)-O(1)	55 29(17)		
Cd(1)-O(7) 2.297(4) N(9)-Cd(1)-O(8) 87.51(18) Cd(1)-O(2) 2.366(5) O(7)-Cd(1)-O(8) 55.14(15) Cd(1)-O(1) 2.391(5) O(2)-Cd(1)-O(8) 115.98(18) Cd(1)-O(8) 2.424(5) O(1)-Cd(1)-O(8) 94.92(18)	Cd(1)-N(9)	2.276(5)	N(1)-Cd(1)-O(8)	151 10(17)		
Cd(1)-O(2) 2.366(5) O(7)-Cd(1)-O(8) 55.14(15) Cd(1)-O(1) 2.391(5) O(2)-Cd(1)-O(8) 115.98(18) Cd(1)-O(8) 2.424(5) O(1)-Cd(1)-O(8) 94.92(18)	Cd(1)-O(7)	2.297(4)	N(9)-Cd(1)-O(8)	87 51(18)		
Cd(1)-O(1) 2.391(5) O(2)-Cd(1)-O(8) 115.98(18) Cd(1)-O(8) 2.424(5) O(1)-Cd(1)-O(8) 94.92(18)	Cd(1)-O(2)	2.257(3)	O(7)-Cd(1)-O(8)	55 14(15)		
Cd(1)-O(8) $2.424(5)$ $O(1)-Cd(1)-O(8)$ $94.92(18)$	Cd(1)-O(1)	2.391(5)	O(2)-Cd(1)-O(8)	115 98(18)		
	Cd(1)-O(1)	2.371(3)	O(1)-Cd(1)-O(8)	94 92(18)		
Cd(2)-O(5)#1 $2,200(5)$ $O(5)#1-Cd(2)-N(4)#2$ $108,55(19)$	Cd(2)-O(5)#1	2 200(5)	O(5)#1-Cd(2)-N(4)#2	108 55(19)		

Table S2. Selected Bond Lengths (Å) and Bond Angles (deg) for 1--6

Cd(2)-N(4)#2	2.246(5)	O(5)#1-Cd(2)-N(12)#3	95.1(2)		
Cd(2)-N(12)#3	2.318(5)	N(4)#2-Cd(2)-N(12)#3	98.3(2)		
Cd(2)-O(13)	2.363(5)	O(5)#1-Cd(2)-O(13)	146.97(18)		
Cd(2)-O(12)	2.371(5)	N(4)#2-Cd(2)-O(13)	99.80(18)		
Cd(3)-O(9)	2.199(5)	N(12)#3-Cd(2)-O(13)	97.3(2)		
Cd(3)-O(11)	2.278(5)	O(5)#1-Cd(2)-O(12)	92.12(18)		
Cd(3)-O(4)#4	2.284(5)	N(4)#2-Cd(2)-O(12)	147.30(19)		
Cd(3)-N(5)	2.294(5)	N(12)#3-Cd(2)-O(12)	104.96(19)		
Cd(3)-O(3)#4	2.404(5)	O(13)-Cd(2)-O(12)	55.10(16)		
Cd(3)-O(10)	2.619(7)	O(9)-Cd(3)-O(11)	109.2(2)		
O(3)-Cd(3)#4	2.404(5)	O(9)-Cd(3)-O(4)#4	142.1(2)		
O(4)-Cd(3)#4	2.284(5)	O(11)-Cd(3)-O(4)#4	91.83(19)		
O(5)-Cd(2)#5	2.200(5)	O(9)-Cd(3)-N(5)	100.8(2)		
N(4)-Cd(2)#2	2.246(5)	O(11)-Cd(3)-N(5)	91.76(19)		
N(12)-Cd(2)#3	2.318(5)	O(4)#4-Cd(3)-N(5)	110.00(19)		
N(1)-Cd(1)-N(9)	97.92(19)	O(9)-Cd(3)-O(3)#4	103.7(2)		
N(1)-Cd(1)-O(7)	96.46(17)	O(11)-Cd(3)-O(3)#4	145.73(18)		
N(9)-Cd(1)-O(7)	107.88(19)	O(4)#4-Cd(3)-O(3)#4	55.24(16)		
N(1)-Cd(1)-O(2)	91.7(2)	N(5)-Cd(3)-O(3)#4	91.4(2)		
N(9)-Cd(1)-O(2)	96.86(18)	O(9)-Cd(3)-O(10)	51.3(2)		
O(7)-Cd(1)-O(2)	152.54(18)	O(11)-Cd(3)-O(10)	90.0(3)		
N(1)-Cd(1)-O(1)	94.27(19)	O(4)#4-Cd(3)-O(10)	99.3(2)		
N(9)-Cd(1)-O(1)	149.95(19)	N(5)-Cd(3)-O(10)	150.6(2)		
O(7)-Cd(1)-O(1)	97.84(17)	O(3)#4-Cd(3)-O(10)	103.4(3)		
Symmetry codes: #1 = x, y-1, z; #2 =	-x+1, -y, -z+1; #3 = -x, -y, -z+1; #	44 = -x, -y, -z+2; #5 = x, y+1, z.			
	Comp	bound 4			
Zn(1)-O(5)#1	1.942(6)	O(5)#1-Zn(1)-O(7)#2	116.4(3)		
Zn(1)-O(1)	1.944(5)	O(1)-Zn(1)-O(7)#2	105.2(2)		
Zn(1)-O(7)#2	1.961(6)	O(5)#1-Zn(1)-N(1)	112.8(3)		
Zn(1)-N(1)	2.010(7)	O(1)-Zn(1)-N(1)	116.6(3)		
Zn(2)-O(1)	1.946(5)	O(7)#2-Zn(1)-N(1)	102.7(3)		
Zn(2)-O(2)	1.964(5)	O(1)-Zn(2)-O(2)	108.6(2)		
Zn(2)-O(6)#2	2.004(6)	O(1)-Zn(2)-O(6)#2	111.6(2)		
Zn(2)-N(4)#1	2.008(6)	O(2)-Zn(2)-O(6)#2	111.9(2)		
O(5)-Zn(1)#3	1.942(6)	O(1)-Zn(2)-N(4)#1	116.7(3)		
O(6)-Zn(2)#2	2.004(6)	O(2)-Zn(2)-N(4)#1	109.2(2)		
O(7)-Zn(1)#2	1.961(6)	O(6)#2-Zn(2)-N(4)#1	98.7(3)		
N(4)-Zn(2)#3	2.008(6)	Zn(1)-O(1)-Zn(2)	112.9(3)		
O(5)#1-Zn(1)-O(1)	103.4(2)				
Symmetry codes: #1 = -x+1, y+1/2, -z+1/2; #2 = -x+1, -y+2, -z; #3 = -x+1, y-1/2, -z+1/2.					
Compound 5					
Cd(1)-N(4)#1	2.277(4)	N(4)#1-Cd(1)-N(1)	90.37(17)		
Cd(1)-O(4)#2	2.290(4)	O(4)#2-Cd(1)-N(1)	97.36(15)		
Cd(1)-O(1)	2.306(4)	O(1)-Cd(1)-N(1)	102.85(16)		

Cd(1)-N(1)	2.321(4)	N(4)#1-Cd(1)-O(2)	100.73(15)	
Cd(1)-O(2)	2.429(4)	O(4)#2-Cd(1)-O(2)	141.17(14)	
Cd(1)-O(3)#2	2.557(4)	O(1)-Cd(1)-O(2)	55.00(13)	
O(3)-Cd(1)#2	2.557(4)	N(1)-Cd(1)-O(2)	99.33(15)	
O(4)-Cd(1)#2	2.290(4)	N(4)#1-Cd(1)-O(3)#2	88.32(15)	
N(4)-Cd(1)#1	2.277(4)	O(4)#2-Cd(1)-O(3)#2	53.90(13)	
N(4)#1-Cd(1)-O(4)#2	113.99(15)	O(1)-Cd(1)-O(3)#2	92.43(14)	
N(4)#1-Cd(1)-O(1)	153.61(17)	N(1)-Cd(1)-O(3)#2	147.03(15)	
O(4)#2-Cd(1)-O(1)	87.19(14)	O(2)-Cd(1)-O(3)#2	113.28(14)	
Symmetry codes: #1 = -x, -y+1, -z+1; #2 = -x, -y, -z; #3 = -x+1, -y, -z.				
	Comj	bound 6		
Cd(1)-O(2)	2.268(3)	O(2)-Cd(1)-O(6)#2	137.30(11)	
Cd(1)-N(1)#1	2.268(3)	N(1)#1-Cd(1)-O(6)#2	95.34(11)	
Cd(1)-N(4)	2.291(3)	N(4)-Cd(1)-O(6)#2	103.49(11)	
Cd(1)-O(6)#2	2.293(3)	O(2)-Cd(1)-O(1)	55.05(10)	
Cd(1)-O(1)	2.486(3)	N(1)#1-Cd(1)-O(1)	93.84(11)	
Cd(1)-O(5)#2	2.505(3)	N(4)-Cd(1)-O(1)	153.20(10)	
O(5)-Cd(1)#3	2.506(3)	O(6)#2-Cd(1)-O(1)	99.15(11)	
O(6)-Cd(1)#3	2.293(3)	O(2)-Cd(1)-O(5)#2	91.46(10)	
N(1)-Cd(1)#1	2.268(3)	N(1)#1-Cd(1)-O(5)#2	149.16(10)	
O(2)-Cd(1)-N(1)#1	117.55(10)	N(4)-Cd(1)-O(5)#2	87.05(11)	
O(2)-Cd(1)-N(4)	98.22(10)	O(6)#2-Cd(1)-O(5)#2	54.05(10)	
N(1)#1-Cd(1)-N(4)	98.10(10)	O(1)-Cd(1)-O(5)#2	94.88(12)	
Symmetry codes: #1 = -x+1, -y+2, -z+1; #2 = -x+2, y+1/2, -z+1/2; #3 = -x+2, y-1/2, -z+1/2.				



Figure S1. (a) Coordination environment of Cd(II) ion in 1 with hydrogen atoms omitted for clarity. Symmetry operator: A = 0.5+x, 1.5-y, -0.5+z; B = 0.5+x, 0.5-y, 0.5+z; (b) Schematic illustrating the 3D topology in complex 1. Color code: purple ball, Cd atom; green stick, *p*-bdc^{2–}linker; yellow stick, pbmb linker.



Figure S2. (a) Coordination environment of Zn(II) ion in **2.** Hydrogen atoms and the free water molecule are omitted for clarity. Symmetry operator: A = 1-x, 2-y, -z; B = x, y, 1+z; C=1+x, y, z; D=1-x, 1-y, -z; E=2-x, 1-y, 1-z.



Figure S3. (a) Coordination environment of Cd(II) ion in **3.** Hydrogen atoms and the free water molecule are omitted for clarity. Symmetry operator: A = x, -1+y, z; B = 1-x, -y, 1-z; C=-x, -y, 1-z; D=-x, -y, 2-z; (b) Schematic illustrating the (2, 3, 4)-connected topology with the topological notation of $(6^{5}.8)_{2}(6^{3})_{2}$. Color code: light blue ball, Cd1 or Cd2 atom; orange ball, Cd3 atom; green ball, 3-connected node.



Figure S4. (a) 2D layer of 4 formed by Zn and 1,2,3-btc³⁻; (b) Schematic illustrating the (3,5)-connected topology with the topological notation of $(3.6^2)(3.6.7)(3.4.5)(3^2.4.5.6^2.7^4)$. Color code: yellow ball, 3-connected node; light blue ball, 5-connected node; pink stick, pbmb linker.



Figure S5. (a) Coordination environment of Cd(II) ion in **5.** Hydrogen atoms are omitted for clarity. Symmetry operator: A = 1-x, -y, -z; B = -x, -y, -z; (b) Schematic illustrating the (3,4)-connected topology with the topological notation of $(4.6^2)(4^2.6^2.8^2)$. Color code: pink stick, pbmb linker; light blue stick, btec⁴⁻ linker.



Figure S6. (a) Coordination environment of Cd(II) ion in **6.** Hydrogen atoms and the free water molecule are omitted for clarity. Symmetry operator: A=-0.5-x, 0.5+y, 1.5-z; B=1-x, 1-y, 2-z; (b) Schematic illustrating the topology with the topological notation of 6^3 . Color code: pink stick, pbmb linker; light blue stick, sdba^{2–} linker.



Figure S7. TGA curves of complexes 1-6.



Complex 3



Complex 6

Figure S8. The simulated (black) and experimental (red) PXRD patterns for compounds 1-6.



Figure S9. The diffuse-reflectance UV-vis spectra for compounds 1–6 and the relative ligands



Figure S10. Kubelka-Munk-transformed diffuse reflectance of complexes 1-6.



Figure S11. Absorption spectra of the MB solution during the decomposition reaction under UV light irradiation with the use of complexes 1-6.