Electronic Supplementary Information

Structural diversity and fluorescent properties of Zn(II)/Cd(II) coordination polymers with a versatile tecton 2-(carboxymethoxy) benzoic acid and N-donor co-ligands

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CrystEngComm

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Table S1 Selected bond lengths (Å) and angles (°) for complexes **1**-**4**

1			
Zn(1)-O(1)	1.9216(19)	Zn(1)-O(4)#1	1.957(2)
Zn(1)-N(3)#2	1.994(2)	Zn(1)-N(1)	2.045(2)
O(1)-Zn(1)-O(4)#1	113.69(9)	O(1)-Zn(1)-N(3)#2	125.15(9)
O(4)#1-Zn(1)-N(3)#2	106.53(10)	O(1)-Zn(1)-N(1)	107.07(9)
O(4)#1-Zn(1)-N(1)	94.93(10)	N(3)#2-Zn(1)-N(1)	104.87(9)

2			
Zn(1)-O(1)	1.929(2)	Zn(1)-O(4)	1.954(2)
Zn(1)-N(1)	2.035(2)	Zn(1)-N(2)#1	2.069(2)
Zn(1)-O(3)	2.317(3)	O(1)-Zn(1)-O(4)	148.33(12)
O(1)-Zn(1)-N(1)	100.02(11)	O(4)-Zn(1)-N(1)	104.34(10)
O(1)-Zn(1)-N(2)#1	97.32(11)	O(4)-Zn(1)-N(2)#1	94.27(9)
N(1)-Zn(1)-N(2)#1	107.66(10)	O(1)-Zn(1)-O(3)	79.41(11)
O(4)-Zn(1)-O(3)	74.18(10)	N(1)-Zn(1)-O(3)	107.58(10)
N(2)#1-Zn(1)-O(3)	144.63(9)		

3			
Zn(1)-O(1)	1.9870(13)	Zn(1)-O(5)#1	1.9390(14)
Zn(1)-N(1)	1.9970(15)	Zn(1)-N(3)	2.0223(16)
O(5)#1-Zn(1)-O(1)	110.00(6)	O(5)#1-Zn(1)-N(1)	123.38(7)
O(1)-Zn(1)-N(1)	106.13(6)	O(5)#1-Zn(1)-N(3)	109.33(7)
O(1)-Zn(1)-N(3)	101.77(6)	N(1)-Zn(1)-N(3)	104.03(7)

4			
Cd(1)-O(6)	2.226(9)	Cd(1)-O(9)#1	2.267(8)
Cd(1)-O(1)	2.278(9)	Cd(1)-O(4)#2	2.328(8)
Cd(1)-O(5)#2	2.550(10)	Cd(1)-O(2)	2.580(8)
Cd(1)-O(10)	2.705(8)	Cd(1)-O(7)	2.784(9)
Cd(2)-N(1)	2.176(10)	Cd(2)-N(4)#3	2.222(10)
Cd(2)-O(7)	2.360(8)	Cd(2)-O(9)	2.339(9)
Cd(2)-O(2)#2	2.426(8)	Cd(2)-O(4)#2	2.503(8)
O(6)-Cd(1)-O(9)#1	98.1(3)	O(6)-Cd(1)-O(1)	115.6(3)
O(9)#1-Cd(1)-O(1)	112.8(3)	O(6)-Cd(1)-O(4)#2	108.3(3)
O(9)#1-Cd(1)-O(4)#2	129.9(3)	O(1)-Cd(1)-O(4)#2	93.3(3)

O(6)-Cd(1)-O(5)#2	155.6(3)	O(9)#1-Cd(1)-O(5)#2	87.1(3)
O(1)-Cd(1)-O(5)#2	83.6(3)	O(4)#2-Cd(1)-O(5)#2	52.9(3)
O(6)-Cd(1)-O(2)	86.4(3)	O(9)#1-Cd(1)-O(2)	74.8(3)
O(1)-Cd(1)-O(2)	53.2(3)	O(4)#2-Cd(1)-O(2)	146.3(3)
O(5)#2-Cd(1)-O(2)	117.9(3)	N(1)-Cd(2)-N(4)#3	176.0(4)
N(1)-Cd(2)-O(7)	90.7(3)	N(4)#3-Cd(2)-O(7)	88.7(3)
N(1)-Cd(2)-O(9)	91.4(3)	N(4)#3-Cd(2)-O(9)	92.5(3)
O(7)-Cd(2)-O(9)	108.0(3)	N(1)-Cd(2)-O(2)#2	92.5(3)
N(4)#3-Cd(2)-O(2)#2	87.9(3)	O(7)-Cd(2)-O(2)#2	174.3(3)
O(9)-Cd(2)-O(2)#2	76.6(3)	N(1)-Cd(2)-O(4)#2	86.4(3)
N(4)#3-Cd(2)-O(4)#2	89.6(3)	O(7)-Cd(2)-O(4)#2	74.2(3)
O(9)-Cd(2)-O(4)#2	176.9(3)	O(2)#2-Cd(2)-O(4)#2	101.2(3)

Symmetry codes: #1: x-1/2, -y-1/2, z-1/2; #2: x-1/2, -y+1/2, z+1/2 for **1**; #1: x+1/2, y+1/2, z for **2**; #1: x, y+1, z for **3**; #1: x, -y+1/2, z-1/2; #2: x, -y+1/2, z+1/2; #3: x-1, y, z for **4**.

Table S2 Hydrogen-bonding lengths (Å) and angles (^{o}) in **1**, **2**, **3** and **4**.

		Complex **1**		
D–H···A	D(D–H)	D(H···A)	D(D···A)	∠DHA
N2–H2A···O1W#1	0.86	1.971	2.828	174.29
O1W–H1WA···O2#2	0.89	2.012	2.878	164.80
O1W–H1WB···O5#2	0.89	1.999	2.875	169.29
		Complex **2**		
O2···O6			2.779	
O5···O6#3			2.908(8)	
O5···O7#4			2.801(1)	
O6···O8#5			2.924(9)	
		Complex **3**		
O1W···O2W			2.783(9)	
O1W···O3W#6			2.902(4)	
O4···O2W			2.825(3)	
		Complex **4**		
O12···O11#7			2.466(1)	
O5···O11#8			2.902(4)	

Symmetry codes: #1: x, y, z-1; #2: x-1/2, -y+1/2, z+1/2; #3: 1/2-x, 1/2+y, 1/2-z; #4: -1+x, y, -1+z; #5: 1/2-x, 1/2-y, 1-z; 6: -1+x, 1+y, z; #8: 1-x, 1-y, -z.

Table S3 The parameters for π···π stacking interactions in **1**, **2**, **3** and **4**.

Complex **1**	
Cg(I) ···*Cg*(J)	*Cg*···*Cg* (Å)
Cg(1) ···*Cg*(2)#1	3.979(2)
Complex **3**	
Cg(3) ···*Cg*(3)#2	3.525(6)
Cg(4) ···*Cg*(4)#3	3.873(5)
Complex **4**	
Cg(5) ···*Cg*(6)#4	3.836(9)

Symmetry codes: #1: 1/2-x, 1/2+y, 1/2-z; #2: -x, 2-y, -z; #3: -x, 1-y, 1-z; #4: 1-x,1-y,1-z.

Cg(1) is the centroid of the N1/C10–C14; *Cg*(2) is the centroid of the N3/C15–C19; *Cg*(3) is the centroid of the N1N2/C10–C12; *Cg*(4) is the centroid of the N3N4/C15–C17; *Cg*(5) is the centroid of the N1N2/C19–C21; *Cg*(6) is the centroid of the C11–C16.

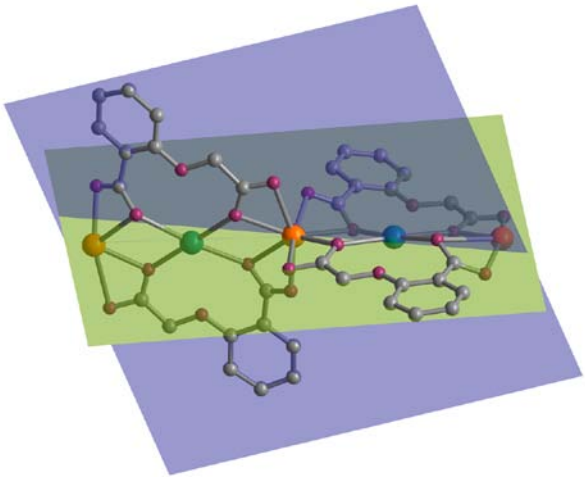


Fig. S1. Dihedral angle of the adjacent platforms in **4**.

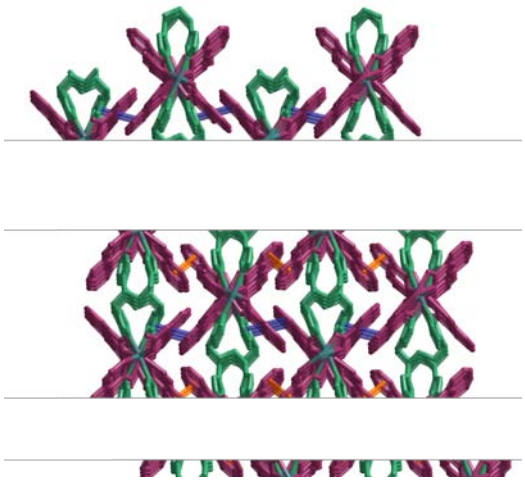
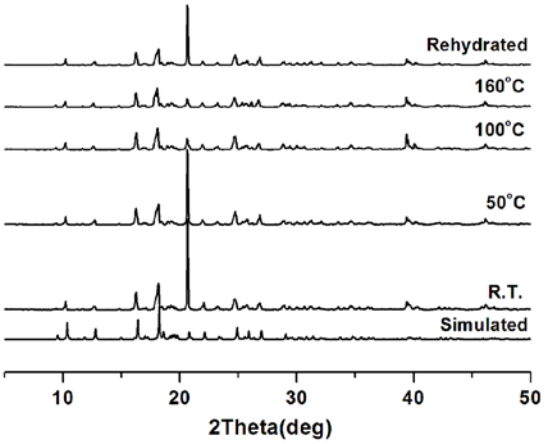
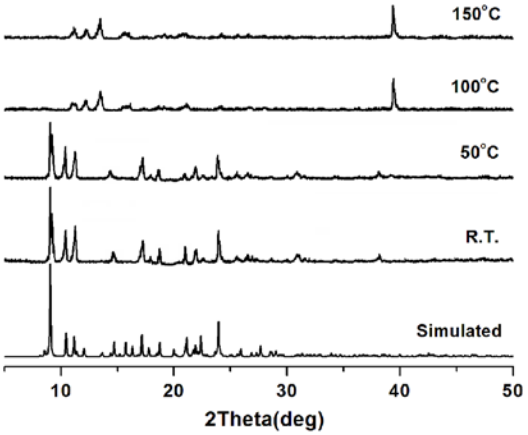


Fig. S2. Perspective view of the 3D network of **4**.



(a)



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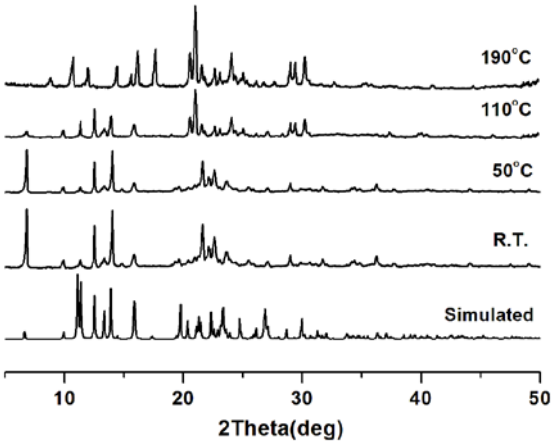

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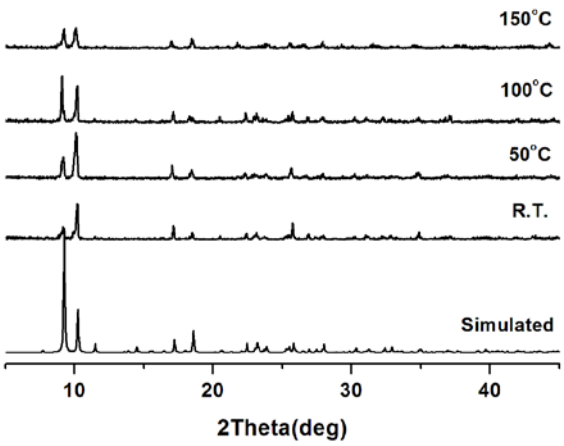

(d)

Fig. S3. The simulated and experimental PXRD patterns for (a) **1**, (b) **2**, (c) **3**, and (d) **4**.

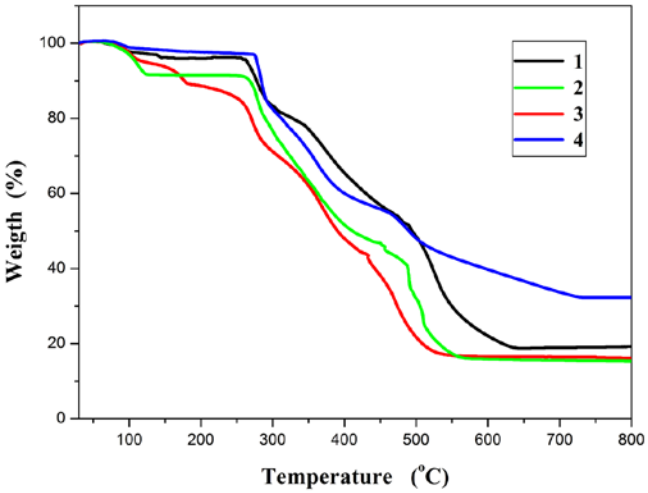

Fig. S4. TGA curves for complexes **1-4**.