Supporting Information

Effects of Solvents and Temperature on the Fluorescence Properties of Cd-Isonicotinic Acid Frameworks Based on Mono-, Bi-, and Trinuclear Cluster Units

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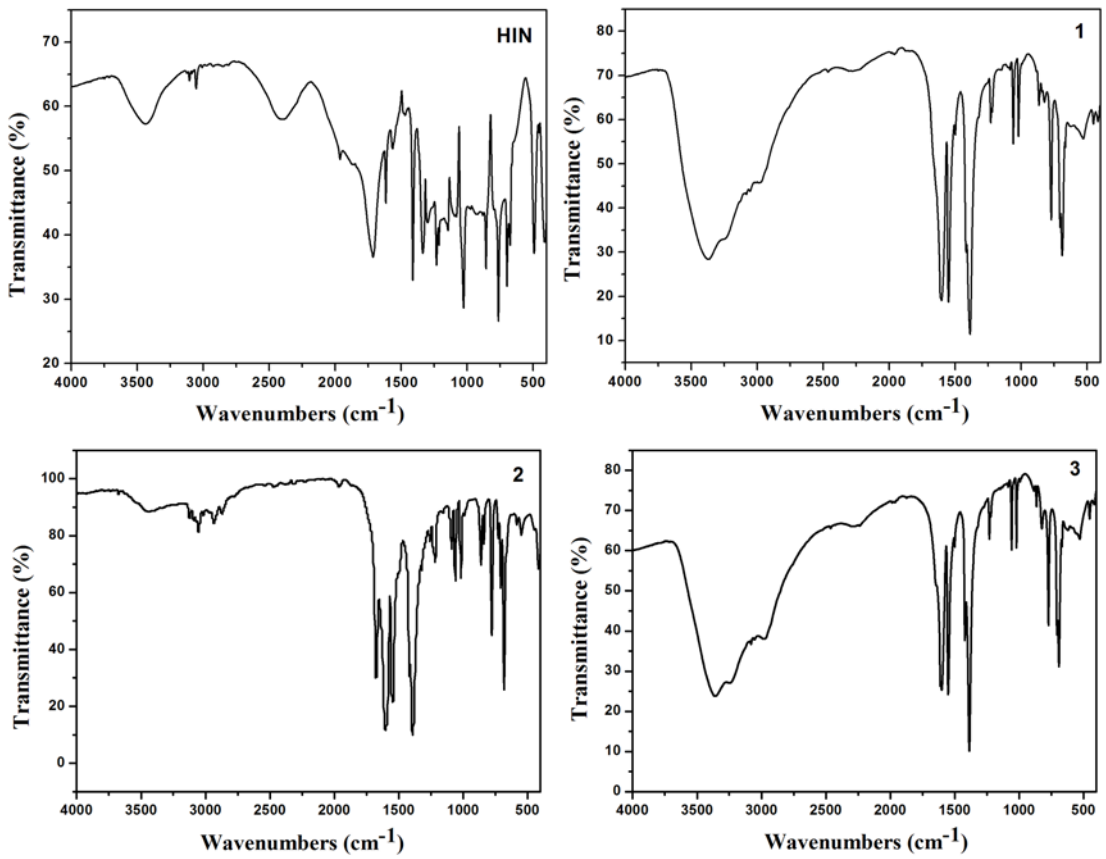

Figure S1. Infrared spectra of coordination polymers **1**–**3** and HIN recorded from a KBr pellet.

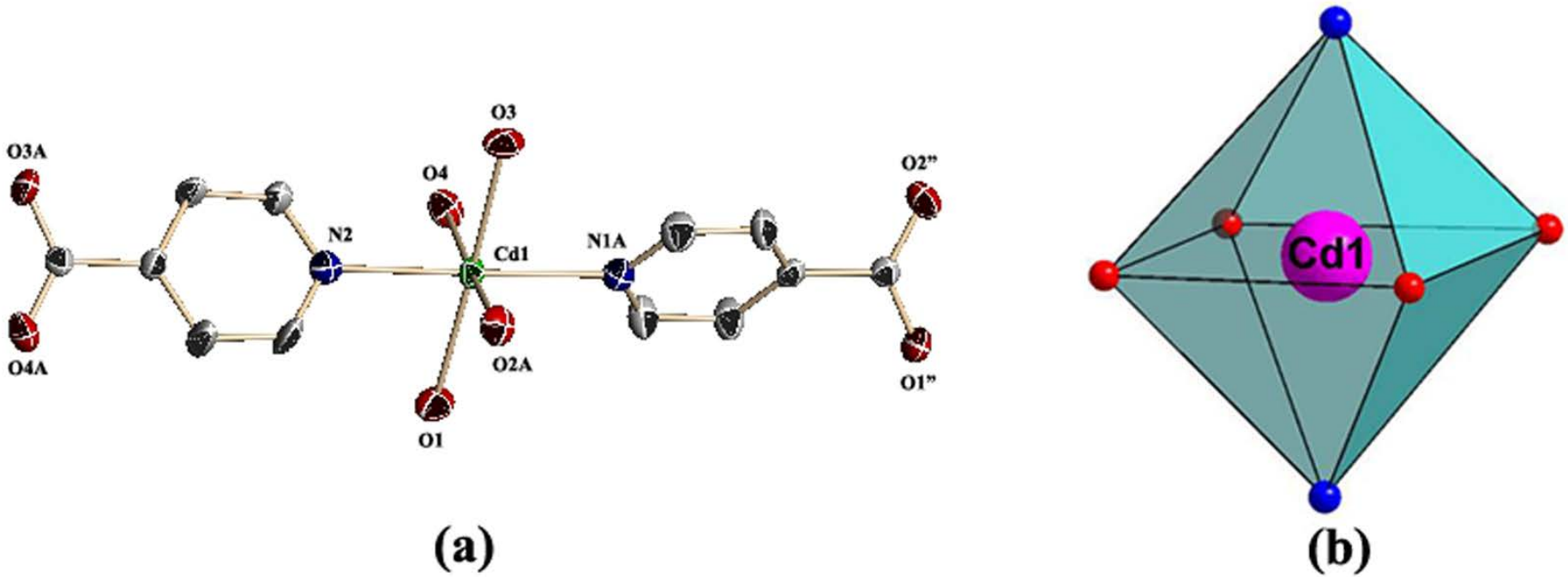

Figure S2. (a) The structural unit of **1** with labeling scheme and 50% thermal ellipsoids (water molecules and hydrogen atoms are omitted for clarity). (b) Polyhedral representation of the coordination sphere of the Cd^{2+} centre, with display octahedron geometry arrangementin in coordination polymer **1**.

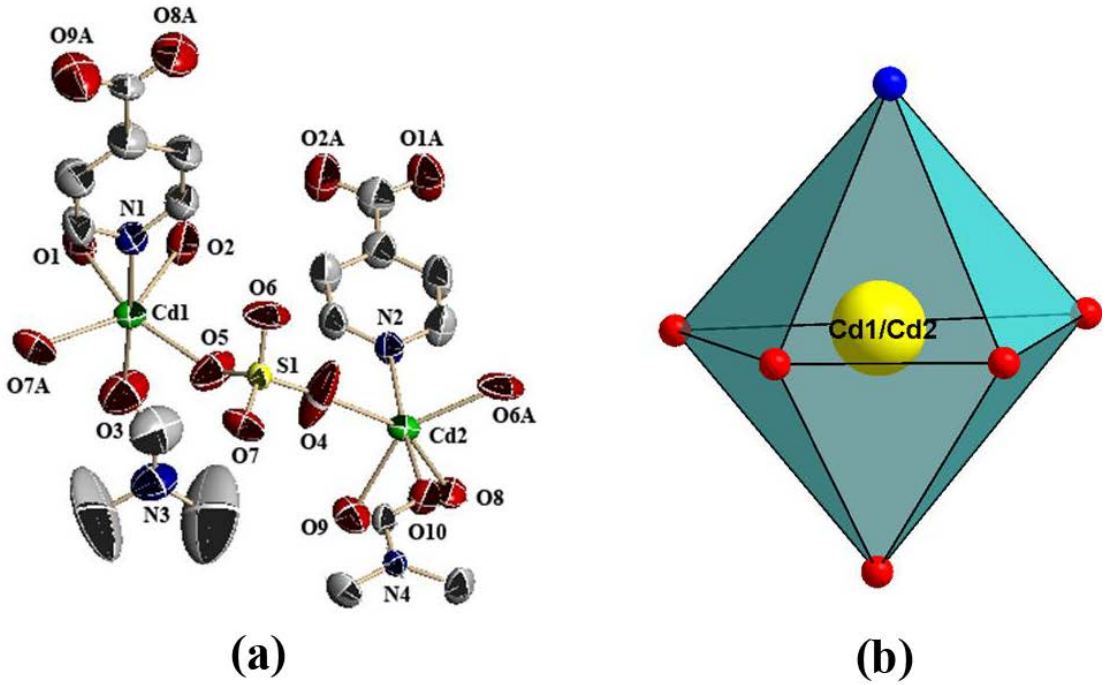

Figure S3. (a) The structural unit of **2** with labeling scheme and 50% thermal ellipsoids (hydrogen atoms are omitted for clarity). (b) Polyhedral representation of the coordination sphere of the Cd^{2+} centre, with display distorted octahedron geometry arrangement in coordination polymer **2**.

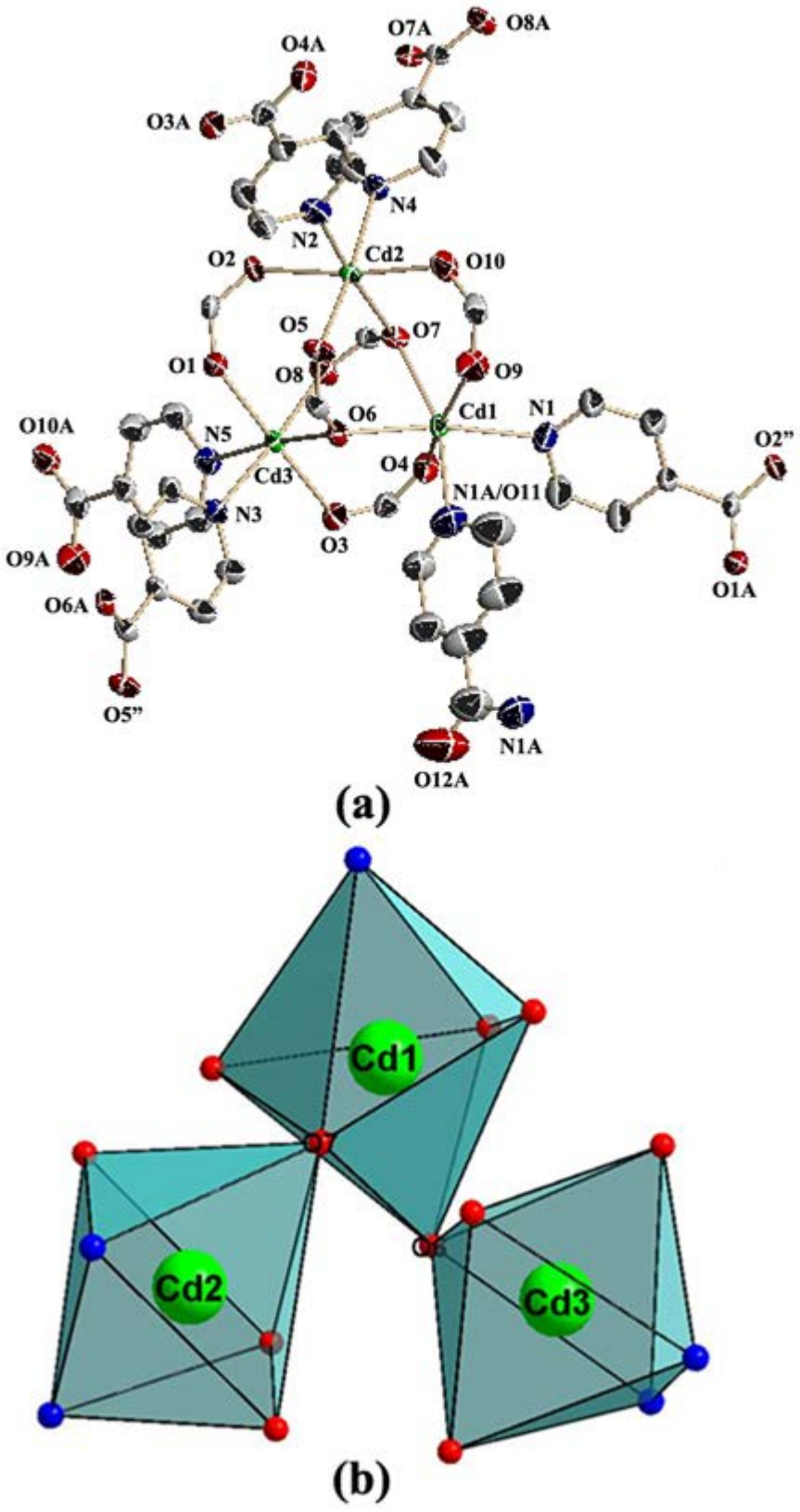

Figure S4. (a) The structural unit of **3** with labeling scheme and 50% thermal ellipsoids (water molecules and hydrogen atoms are omitted for clarity). (b) Polyhedral representation of the coordination sphere of the Cd^{2+} centre in coordination polymer **3**.

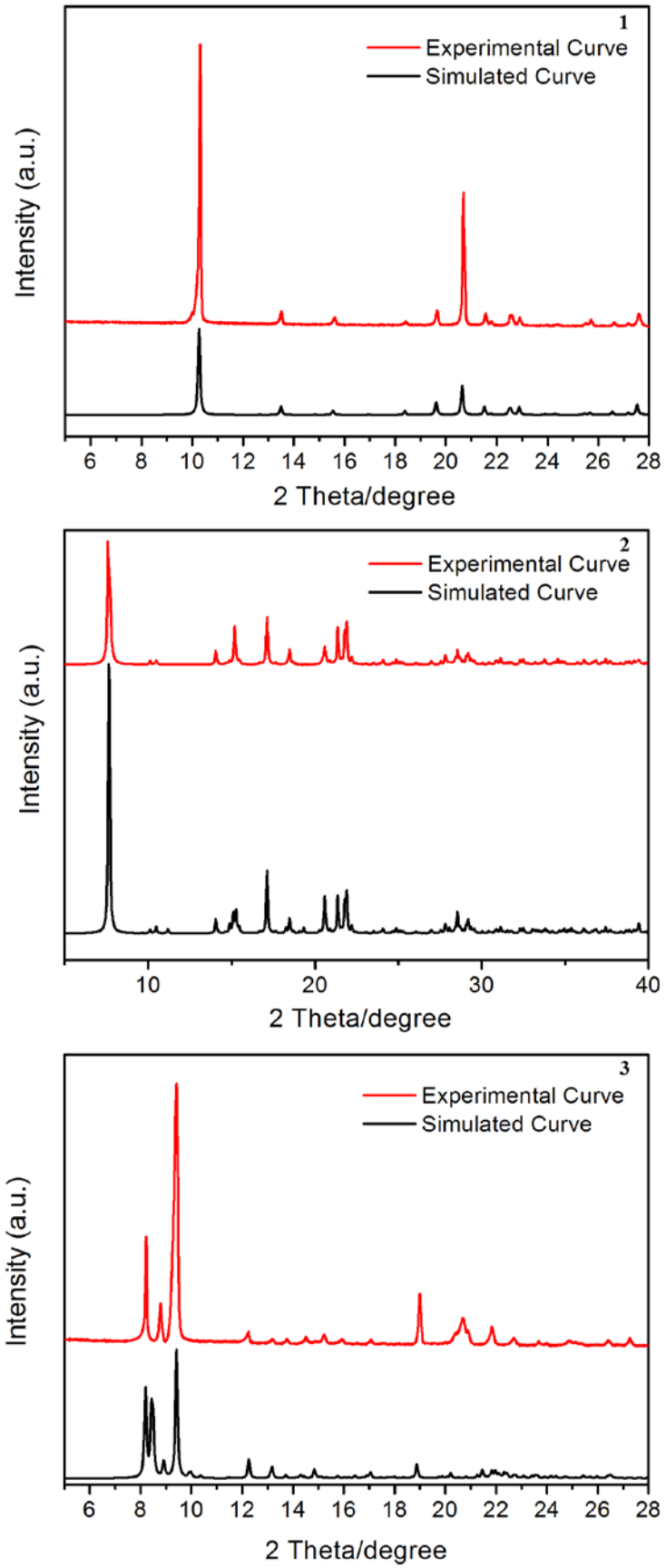

Figure S5. The PXRD contrast curves of coordination polymers **1**–**3**.

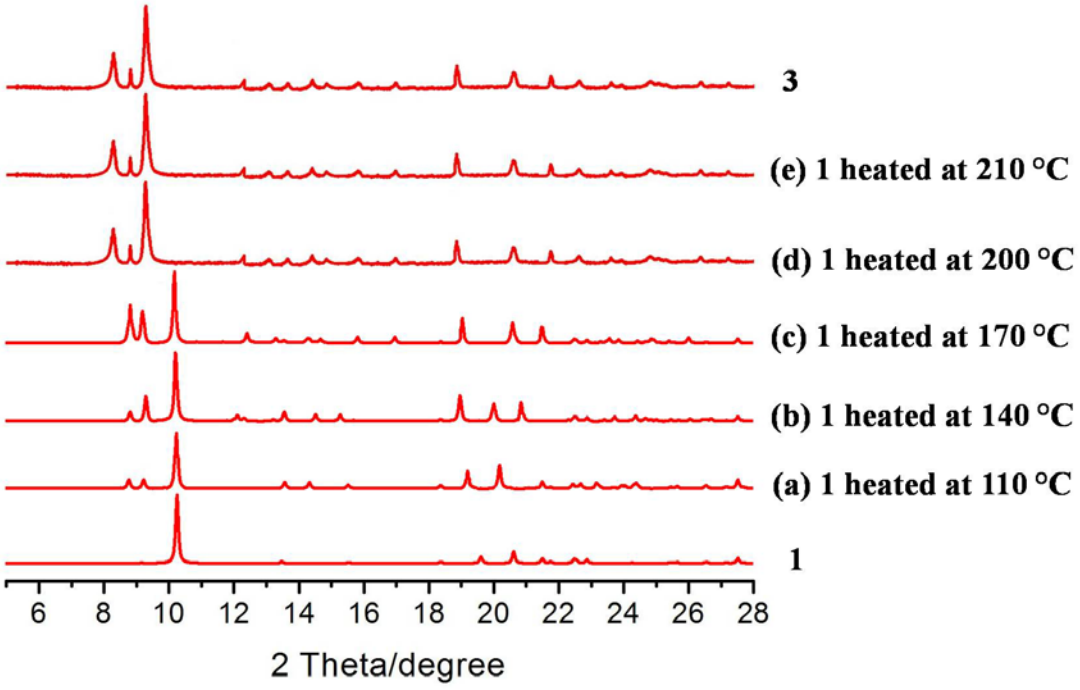

Figure S6. The PXRD patterns of **1** at different temperatures: (a) **1** heated at 110 °C, (b) **1** heated at 140 °C, (c) **1** heated at 170 °C, (d) **1** heated at 200 °C, (e) **1** heated at 210 °C.

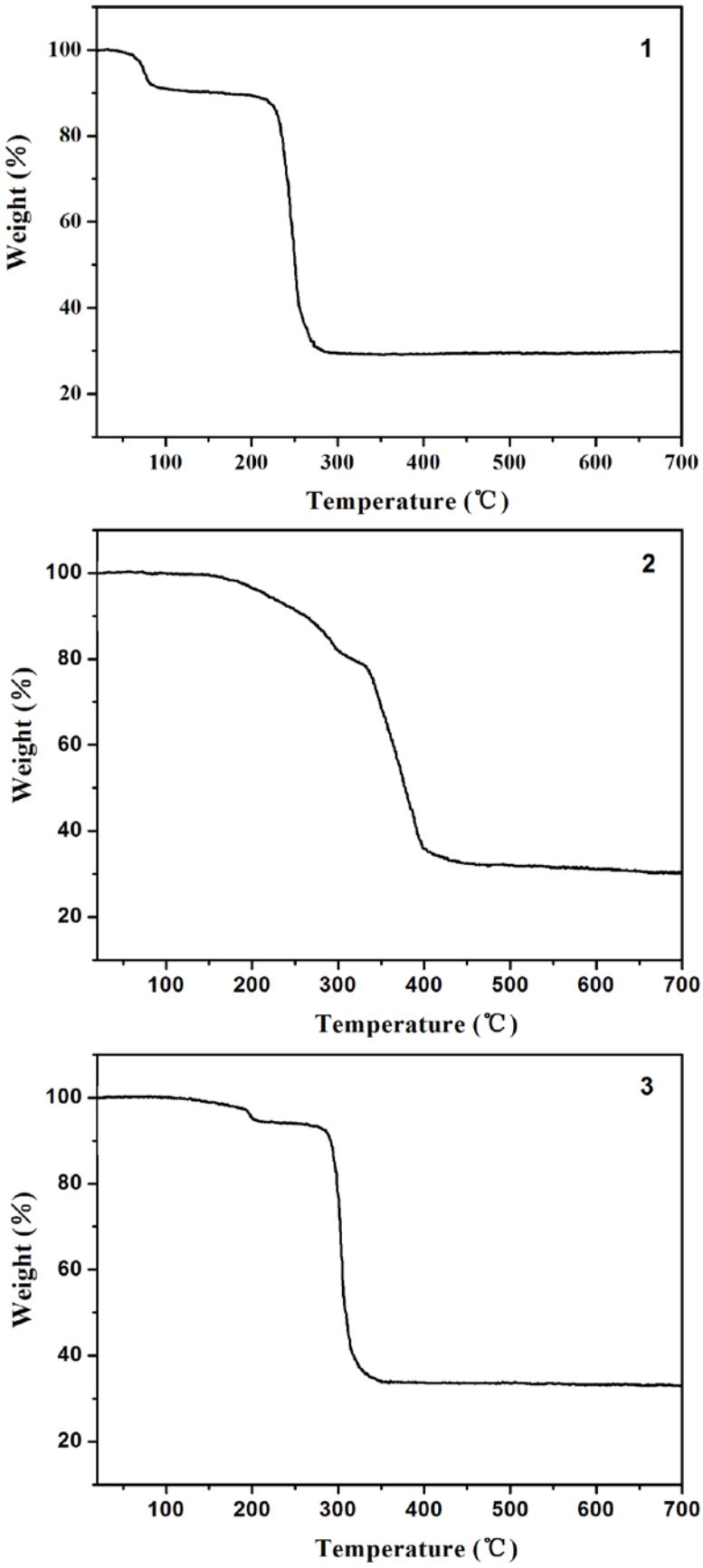

Figure S7. The TGA curves of coordination polymers **1**–**3**.

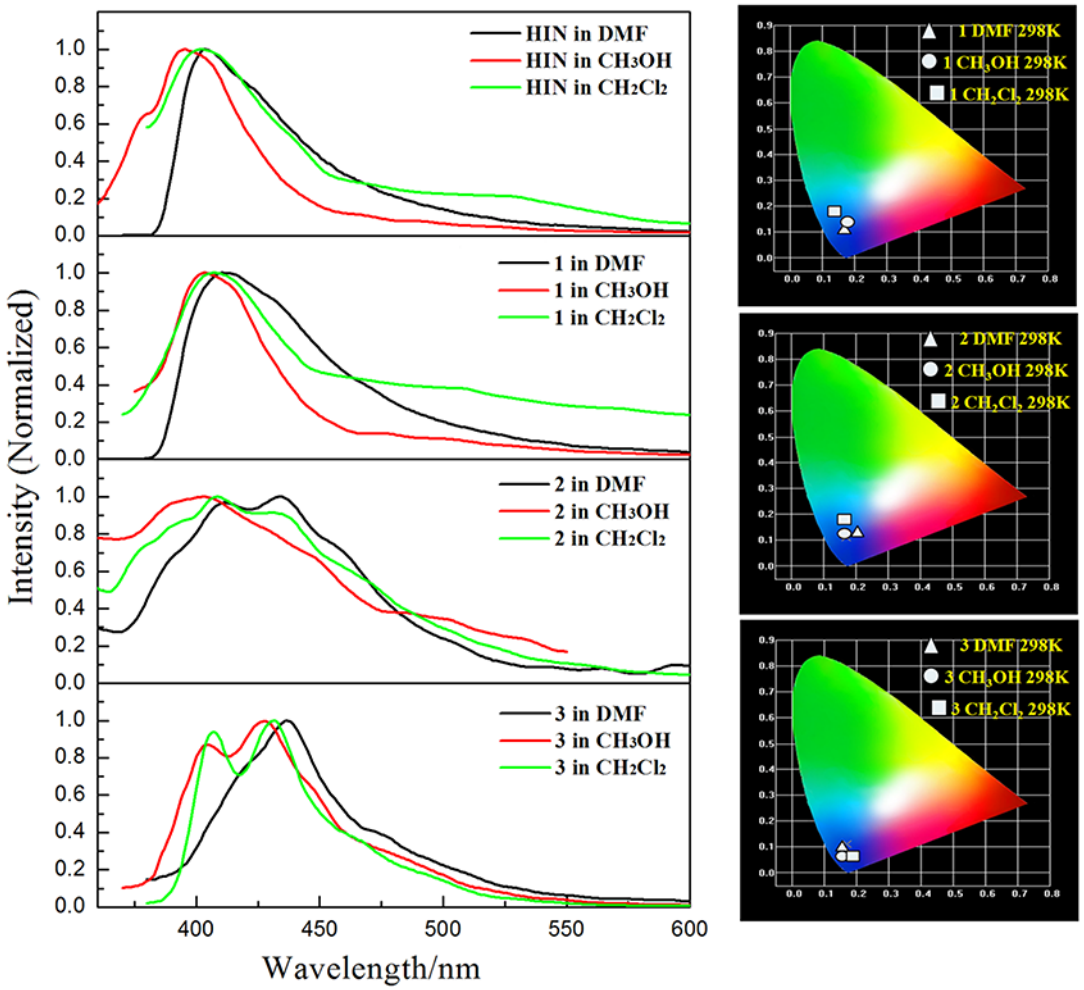

Figure S8. Normalized emission spectra of coordination polymers **1**–**3** and HIN in DMF, CH_3OH and CH_2Cl_2 solutions (concentration: (M) ≈ 10^{-5} M) at 298 K and the corresponding color coordinate diagram of emission.

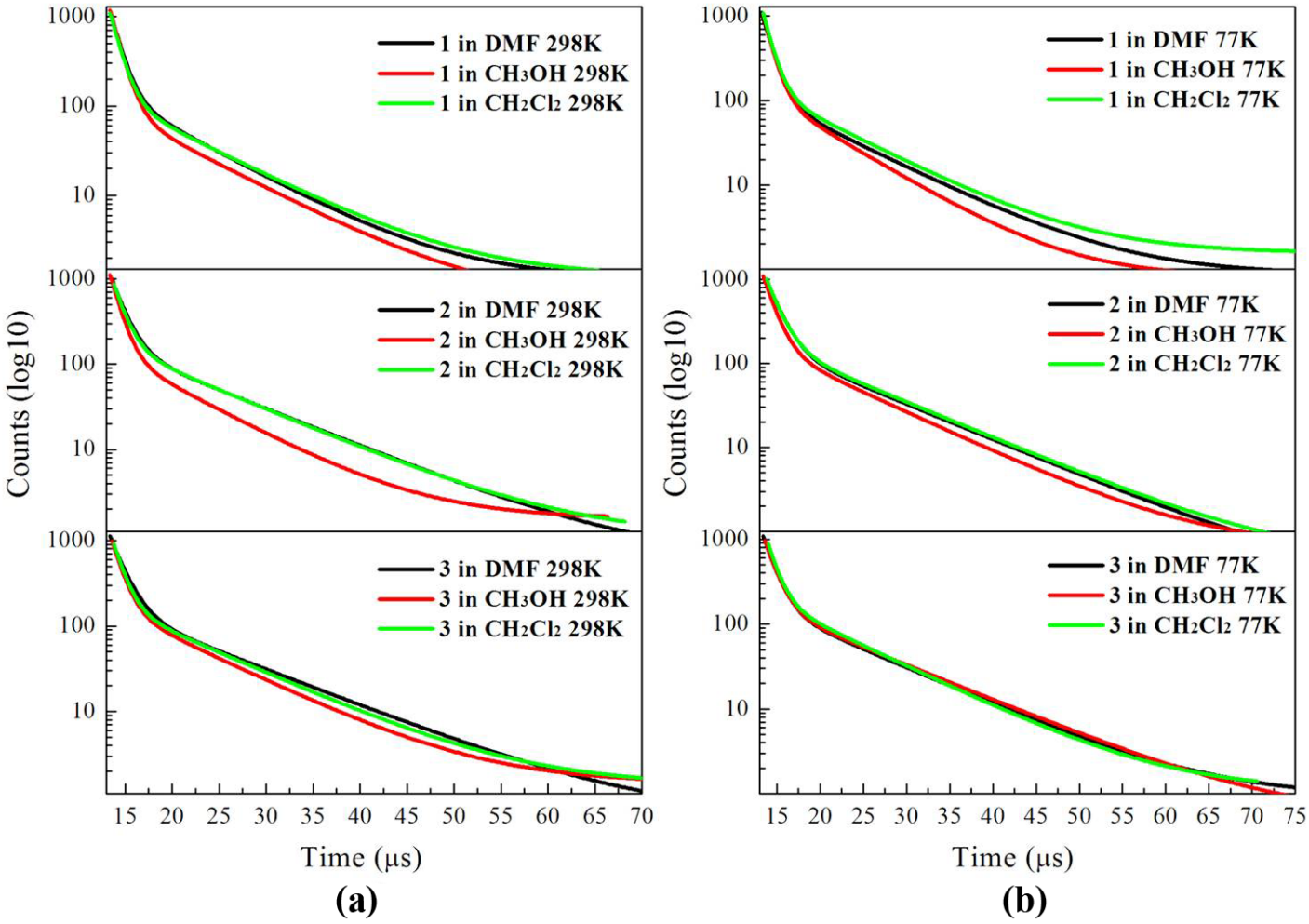

Figure S9. The decay curves of coordination polymers **1**–**3** measured in DMF, CH_3OH and CH_2Cl_2 solutions at 298 K (a) and 77 K (b).

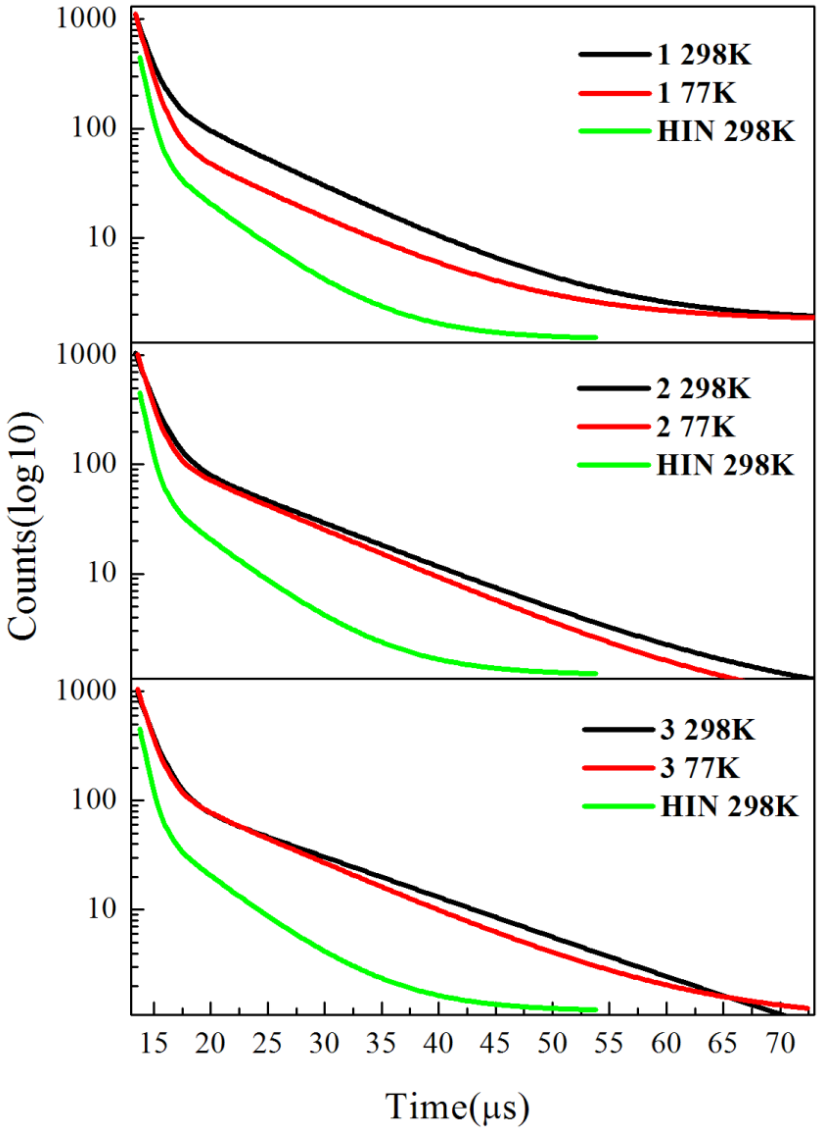

Figure S10. The decay curves of coordination polymers **1**–**3** at 298 K, 77 K and HIN at 298 K in solid state.

Table S1

Selected bond distance (Å) and angles (˚) in coordination polymer **1**.

1					
Cd(1)-O(1)	2.290(7)	Cd(1)-O(3)	2.283(7)	Cd(1)-N(2)	2.305(8)
Cd(1)-O(2)#1	2.341(7)	Cd(1)-O(4)	2.334(7)	Cd(1)-N(1)#2	2.359(8)
O(1)-C(6)	1.251(11)	O(2)-C(6)	1.251(11)	O(2)-Cd(1)#1	2.341(7)
O(3)-C(12)	1.249(11)	O(4)-C(12)#3	1.262(11)	N(1)-C(4)	1.336(13)
N(1)-C(3)	1.330(13)	N(1)-Cd(1)#4	2.359(8)	N(2)-C(9)	1.319(14)
N(2)-C(10)	1.318(13)	C(1)-C(5)	1.389(14)	C(1)-C(2)	1.380(14)
C(1)-C(6)	1.513(12)	C(2)-C(3)	1.379(14)	C(4)-C(5)	1.391(14)
C(7)-C(8)	1.376(14)	C(7)-C(11)	1.388(13)	C(7)-C(12)#5	1.513(12)
C(8)-C(9)	1.393(15)	C(10)-C(11)	1.389(13)	C(12)-O(4)#3	1.262(11)
O(1)-Cd(1)-O(3)	177.6(3)	O(1)-Cd(1)-N(2)	82.9(3)	O(1)-Cd(1)-N(1)	96.4(3)
O(1)-Cd(1)-O(2)#1	96.4(3)	O(3)-Cd(1)-O(2)#1	82.2(3)	N(2)-Cd(1)-O(2)#1	88.7(3)
O(1)-Cd(1)-O(4)	88.1(3)	O(3)-Cd(1)-O(4)	93.2(3)	N(2)-Cd(1)-O(4)	90.7(3)
O(2)#1-Cd(1)-O(4)	175.4(3)	O(1)-Cd(1)-N(1)#2	96.4(3)	O(3)-Cd(1)-N(1)#2	85.8(3)
N(2)-Cd(1)-N(1)#2	175.8(3)	O(2)#1-Cd(1)-N(1)#2	95.4(3)	O(4)-Cd(1)-N(1)#2	85.1(3)
C(6)-O(2)-Cd(1)#1	129.2(6)	C(12)-O(3)-Cd(1)	137.5(7)	C(12)#3-O(4)-Cd(1)	143.3(6)
C(4)-N(1)-C(3)	119.1(9)	C(4)-N(1)-Cd(1)#4	120.6(7)	C(3)-N(1)-Cd(1)#4	120.3(7)
C(9)-N(2)-C(10)	118.4(9)	C(9)-N(2)-Cd(1)	122.3(7)	C(10)-N(2)-Cd(1)	122.3(7)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x+1,y+1/2,-z+1/2 #3 -x+2,-y+1,-z+1 #4 -x+1,y-1/2,-z+1/2
#5 -x+2,y-1/2,-z+3/2

Selected bond distance (Å) and angles (˚) in coordination polymer **2**.

2					
Cd(1)-O(1)	2.309(7)	Cd(1)-O(3)	2.315(8)	Cd(1)-O(7)	2.256(7)
Cd(1)-O(2)	2.419(6)	Cd(1)-O(5)	2.204(7)	Cd(1)-N(1)	2.319(6)
Cd(2)-O(4)#2	2.190(8)	Cd(2)-O(6)#3	2.275(8)	Cd(2)-O(8)	2.334(7)
Cd(2)-O(9)	2.423(7)	Cd(2)-O(10)	2.279(7)	Cd(2)-N(2)	2.307(6)
S(1)-O(4)	1.414(8)	S(1)-O(5)	1.453(7)	S(1)-O(6)	1.437(8)
S(1)-O(7)	1.445(7)	O(1)-C(7)	1.226(10)	O(2)-C(7)	1.250(10)
O(3)-C(13)	1.080(16)	O(8)-C(1)	1.227(12)	O(9)-C(1)	1.247(12)
O(10)-C(16)	1.224(11)	N(1)-C(4)	1.323(11)	N(1)-C(5)	1.352(11)
N(2)-C(12)	1.325(10)	N(2)-C(11)	1.342(10)	N(3)-C(13)	1.324(16)
N(3)-C(15)	1.43(2)	N(3)-C(14)	1.45(2)	N(4)-C(16)	1.317(12)
N(4)-C(18)	1.450(12)	N(4)-C(17)	1.450(13)	C(1)-C(2)	1.524(11)
C(2)-C(6)	1.379(13)	C(2)-C(3)	1.398(12)	C(3)-C(4)	1.377(12)
C(5)-C(6)	1.371(12)	C(7)-C(8)	1.501(11)	C(8)-C(9)	1.390(11)
C(8)-C(10)	1.391(12)	C(9)-C(11)#5	1.382(11)	C(10)-C(12)#5	1.377(12)
O(5)#1-Cd(1)-O(7)	116.0(3)	O(5)#1-Cd(1)-O(1)	153.6(3)	O(7)-Cd(1)-O(1)	89.0(2)
O(5)#1-Cd(1)-O(3)	83.4(3)	O(7)-Cd(1)-O(3)	88.1(3)	O(1)-Cd(1)-O(3)	89.6(3)
O(5)#1-Cd(1)-N(1)	97.8(3)	O(7)-Cd(1)-N(1)	88.9(3)	O(1)-Cd(1)-N(1)	90.6(3)
O(3)-Cd(1)-N(1)	176.9(3)	O(5)#1-Cd(1)-O(2)	99.9(3)	O(7)-Cd(1)-O(2)	143.6(3)
O(1)-Cd(1)-O(2)	54.6(2)	O(3)-Cd(1)-O(2)	90.5(3)	N(1)-Cd(1)-O(2)	92.1(3)
O(4)#2-Cd(2)-O(6)#3	119.7(5)	O(4)#2-Cd(2)-O(10)	89.5(3)	O(6)#3-Cd(2)-O(10)	84.2(3)
O(4)#2-Cd(2)-N(2)	89.2(3)	O(6)#3-Cd(2)-N(2)	89.8(3)	O(10)-Cd(2)-N(2)	172.2(3)
O(4)#2-Cd(2)-O(8)	149.9(5)	O(6)#3-Cd(2)-O(8)	90.4(3)	O(10)-Cd(2)-O(8)	94.5(3)
N(2)-Cd(2)-O(8)	90.5(3)	O(4)#2-Cd(2)-O(9)	95.9(5)	O(6)#3-Cd(2)-O(9)	143.4(3)
O(10)-Cd(2)-O(9)	88.2(3)	N(2)-Cd(2)-O(9)	99.5(3)	O(8)-Cd(2)-O(9)	54.5(2)
O(4)-S(1)-O(6)	108.8(8)	O(4)-S(1)-O(7)	104.7(6)	O(6)-S(1)-O(7)	110.5(6)
O(4)-S(1)-O(5)	110.0(7)	O(6)-S(1)-O(5)	109.9(4)	O(7)-S(1)-O(5)	112.8(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x+1,-y+1,-z+1 #3 x-1,y,z+1 #4 x+1,y,z-1 #5 -x,-y+2,-z+1

Selected bond distance (Å) and angles (˚) in coordination polymer **3**.

3					
Cd(1)-O(9)	2.220(3)	Cd(1)-O(4)	2.265(3)	Cd(1)-O(11)	2.297(4)
Cd(1)-O(6)	2.335(3)	Cd(1)-O(7)	2.401(2)	Cd(1)-N(1)	2.376(4)
Cd(2)-O(10)	2.240(3)	Cd(2)-O(2)	2.258(2)	Cd(2)-O(5)	2.269(2)
Cd(2)-O(7)	2.402(3)	Cd(2)-N(2)	2.353(3)	Cd(2)-N(4)	2.347(3)
Cd(3)-O(1)	2.241(3)	Cd(3)-O(3)	2.246(3)	Cd(3)-O(8)	2.272(2)
Cd(3)-O(6)	2.404(2)	Cd(3)-N(3)	2.337(3)	Cd(3)-N(5)	2.357(3)
O(8)-C(19)	1.237(4)	O(6)-C(13)	1.264(5)	O(7)-C(19)	1.284(4)
O(3)-C(7)	1.236(5)	O(5)-C(13)	1.243(5)	O(1)-C(1)	1.254(5)
O(2)-C(1)	1.261(4)	O(10)-C(25)	1.243(5)	N(4)-C(23)	1.344(5)
N(4)-C(24)	1.341(4)	O(4)-C(7)	1.250(4)	N(5)-C(29)	1.337(5)
N(5)-C(27)	1.334(5)	N(3)-C(17)	1.339(5)	N(3)-C(18)	1.338(5)
C(16)-C(17)#1	1.379(5)	C(21)-C(24)#2	1.380(5)	C(26)-C(28)#3	1.383(6)
O(9)-Cd(1)-O(4)	162.0(12)	O(9)-Cd(1)-O(11)	100.5(4)	O(4)-Cd(1)-O(11)	92.3(4)
O(9)-Cd(1)-O(6)	95.5(3)	O(4)-Cd(1)-O(6)	98.6(10)	O(11)-Cd(1)-O(6)	83.1(4)
O(9)-Cd(1)-N(1)	86.6(4)	O(4)-Cd(1)-N(1)	81.6(3)	O(11)-Cd(1)-N(1)	86.0(4)
O(6)-Cd(1)-N(1)	169.1(3)	O(9)-Cd(1)-O(7)	89.5(3)	O(4)-Cd(1)-O(7)	82.0(3)
O(11)-Cd(1)-O(7)	161.3(4)	O(6)-Cd(1)-O(7)	80.2(2)	N(1)-Cd(1)-O(7)	110.5(3)
O(10)-Cd(2)-O(2)	172.7(3)	O(10)-Cd(2)-O(5)	94.2(3)	O(2)-Cd(2)-O(5)	90.5(3)
O(10)-Cd(2)-N(4)	87.2(3)	O(2)-Cd(2)-N(4)	87.5(3)	O(5)-Cd(2)-N(4)	173.4(2)
O(1)-Cd(3)-O(3)	178.5(3)	O(1)-Cd(3)-O(8)	88.8(3)	O(3)-Cd(3)-O(8)	89.5(3)
O(8)-Cd(3)-N(3)	174.7(3)	O(3)-Cd(3)-N(5)	86.7(3)	N(5)-Cd(3)-O(6)	173.0(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+1,-y+1,-z #3 x+1,y+1,z