Electronic Supplementary Information (ESI)

Substituent effect of *R*-isophthalates (*R* = –H, –CH_3, –OCH_3, –*t*Bu, –OH, and –NO_2) on the construction of Cd^{II} coordination polymers incorporating a dipyridyl tecton 2,5-bis(3-pyridyl)-1,3,4-oxadiazole

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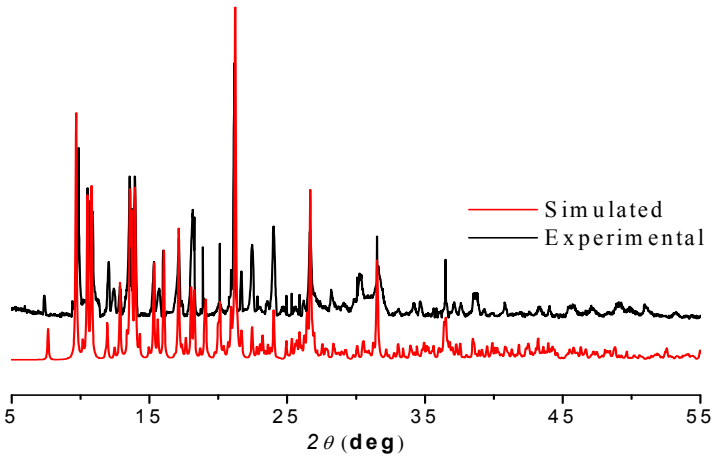
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Experimental
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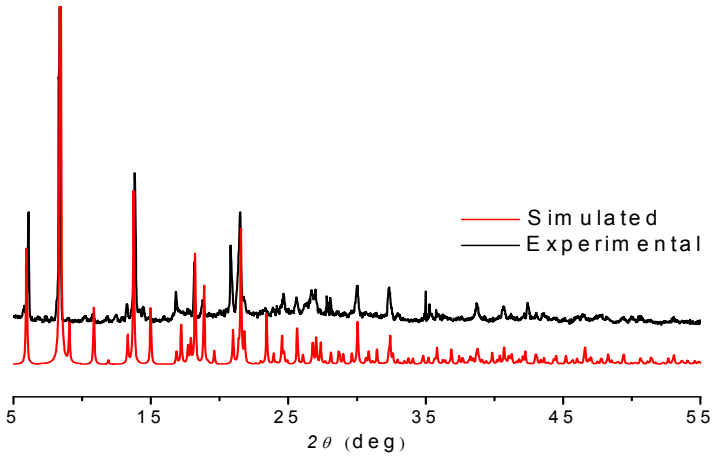
2θ (deg)

(a)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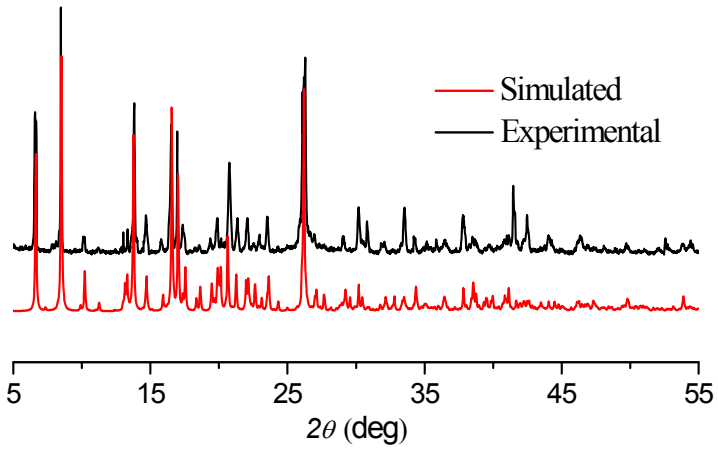
(b)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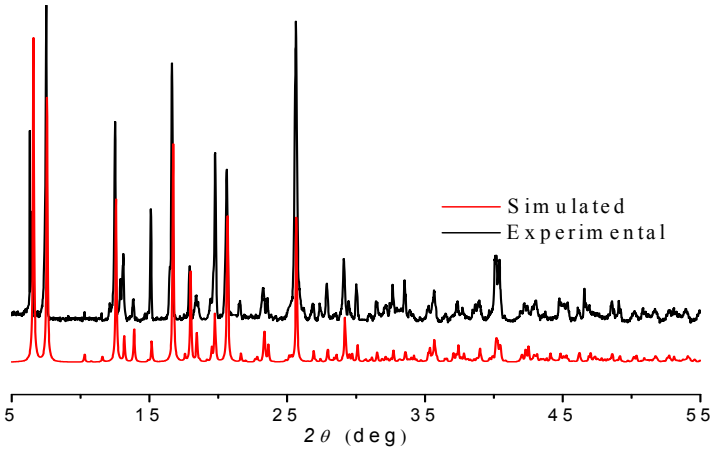
(c)



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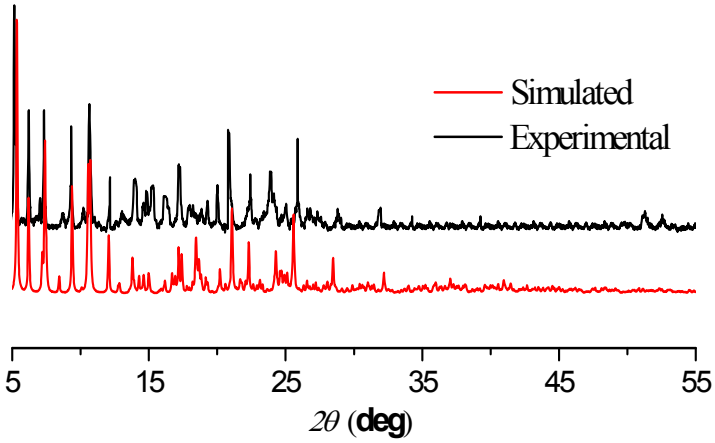

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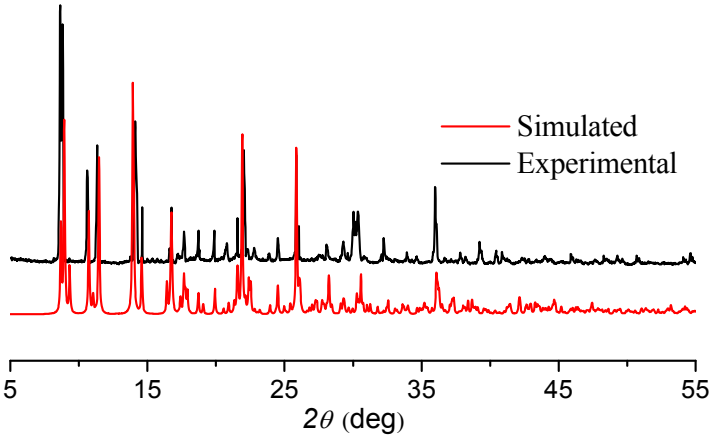
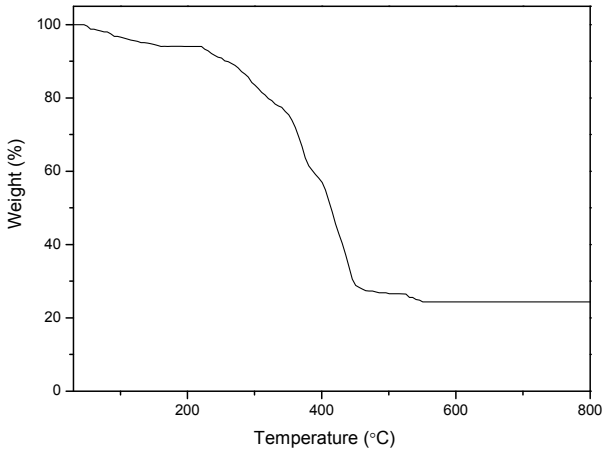


(f)

Fig. S1 Powder X-ray diffraction (PXRD) patterns for complexes **1**–**6** (**a**–**f**).


Weight (%)
Temperature (°C)
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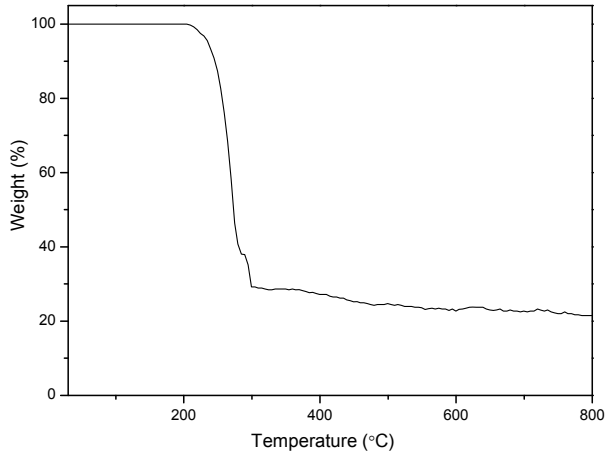
20
40
60
80
100
200
400
600
800

(a)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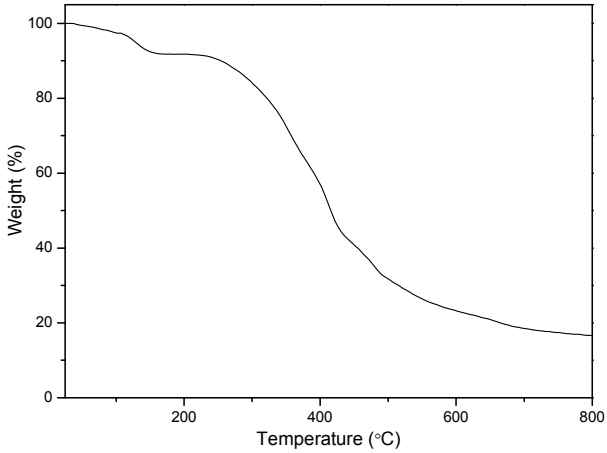
(b)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80
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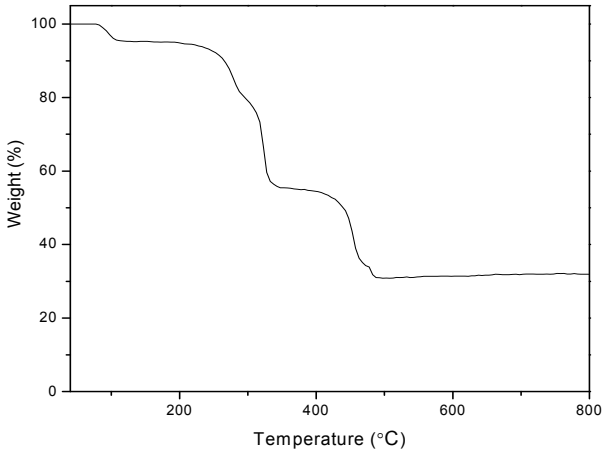
200
400
600
800

(c)



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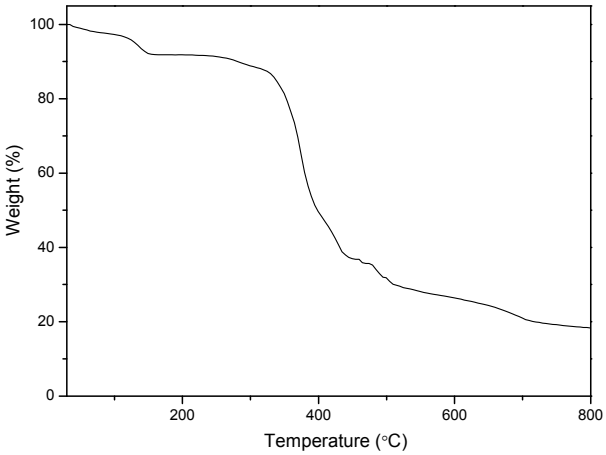

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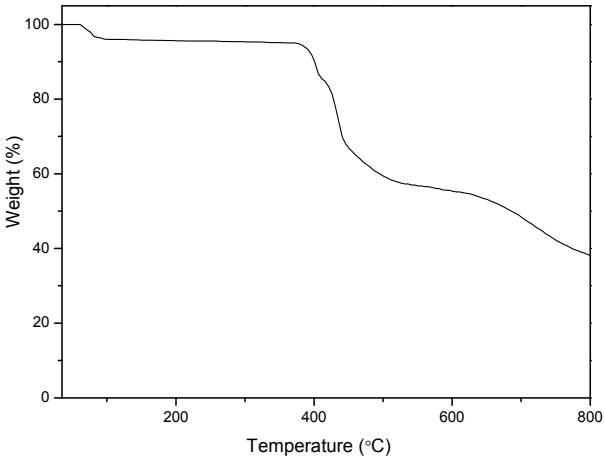

(f)

Fig. S2 TGA curves for complexes **1**–**6** (**a**–**f**).

Table S1 Selective bond lengths (Å) and angles (º) for complexes **1**–**6**

1

Cd1–O3	2.170(3)	Cd1–N1	2.335(3)
Cd1–O11	2.338(3)	Cd1–O5A	2.378(3)
Cd1–O6A	2.397(3)	Cd1–N5	2.408(3)
Cd2–O12	2.298(3)	Cd2–O10A	2.305(3)
Cd2–O7	2.322(3)	Cd2–N8	2.355(3)
Cd2–N4	2.383(3)	Cd2–O9A	2.545(3)
Cd2–O8	2.682(4)		
O3–Cd1–N1	103.1(1)	O3–Cd1–O11	123.3(1)
N1–Cd1–O11	90.6(1)	O3–Cd1–O5A	146.2(1)
N1–Cd1–O5A	82.9(1)	O11–Cd1–O5A	89.5(1)
O3–Cd1–O6A	91.7(1)	N1–Cd1–O6A	91.2(1)
O11–Cd1–O6A	143.5(1)	O5A–Cd1–O6A	54.67(9)
O3–Cd1–N5	90.5(1)	N1–Cd1–N5	166.2(1)
O11–Cd1–N5	83.9(1)	O5A–Cd1–N5	84.4(1)
O6A–Cd1–N5	85.9(1)	O12–Cd2–O10A	139.8(1)
O12–Cd2–O7	131.6(1)	O10A–Cd2–O7	87.7(1)
O12–Cd2–N8	91.3(1)	O10A–Cd2–N8	100.1(1)
O7–Cd2–N8	87.6(1)	O12–Cd2–N4	84.0(1)
O10A–Cd2–N4	90.2(1)	O7–Cd2–N4	87.7(1)
N8–Cd2–N4	168.5(1)	O12–Cd2–O9A	89.3(1)
O10A–Cd2–O9A	53.5(1)	O7–Cd2–O9A	138.9(1)
N8–Cd2–O9A	86.8(1)	N4–Cd2–O9A	103.6(1)
O8–Cd2–O12	81.2(1)	O8–Cd2–O10A	138.5(1)
O8–Cd2–O7	50.9(1)	O8–Cd2–N8	80.2(1)
O8–Cd2–N4	88.7(1)	O8–Cd2–O9A	163.7(1)

2

Cd1–O4A	2.229(4)	Cd1–O5B	2.263(5)
Cd1–N4B	2.322(6)	Cd1–O3	2.371(5)
Cd1–N1	2.377(6)	Cd1–O2	2.403(4)
O4A–Cd1–O5B	125.8(2)	O4A–Cd1–N4B	96.8(2)
O5B–Cd1–N4B	86.4(2)	O4A–Cd1–O3	88.8(2)
O5B–Cd1–O3	145.4(2)	N4B–Cd1–O3	91.3(2)
O4A–Cd1–N1	90.0(2)	O5B–Cd1–N1	86.6(2)
N4B–Cd1–N1	172.3(2)	O3–Cd1–N1	92.5(2)
O4A–Cd1–O2	143.1(2)	O5B–Cd1–O2	90.8(2)
N4B–Cd1–O2	88.4(2)	O3–Cd1–O2	54.5(2)
N1–Cd1–O2	88.5(2)		

3

Cd1–O2	2.234(4)	Cd1–O3A	2.251(4)
Cd1–O26	2.328(4)	Cd1–N1	2.346(5)
Cd1–O25	2.354(4)	Cd1–O4A	2.569(4)
Cd1–O1	2.655(5)	Cd2–O7	2.213(4)
Cd2–O9B	2.273(4)	Cd2–N4	2.324(5)
Cd2–O27	2.369(4)	Cd2–O31	2.451(4)
Cd2–O8B	2.479(4)	Cd2–O6	2.705(4)
Cd3–O19C	2.269(4)	Cd3–O12	2.283(4)
Cd3–O28	2.309(4)	Cd3–O29	2.334(4)
Cd3–N7	2.366(5)	Cd3–O20C	2.524(4)
Cd3–O13	2.548(4)	Cd4–O18	2.259(3)
Cd4–O14	2.308(4)	Cd4–O30	2.324(4)
Cd4–N9	2.331(4)	Cd4–N5	2.342(5)
Cd4–O15	2.543(4)	Cd4–O17	2.665(5)

O2–Cd1–O3A	141.0(2)	O2–Cd1–O26	85.8(2)
O3A–Cd1–O26	94.1(2)	O2–Cd1–N1	136.1(2)
O3A–Cd1–N1	82.9(2)	O26–Cd1–N1	92.2(2)
O2–Cd1–O25	90.6(2)	O3A–Cd1–O25	91.9(2)
O26–Cd1–O25	173.8(2)	N1–Cd1–O25	86.9(2)
O2–Cd1–O4A	88.1(1)	O3A–Cd1–O4A	53.0(2)
O26–Cd1–O4A	94.6(2)	N1–Cd1–O4A	135.7(2)
O25–Cd1–O4A	90.4(1)	O1–Cd1–O2	52.3(2)
O1–Cd1–O3A	166.5(2)	O1–Cd1–O26	84.0(1)
O1–Cd1–N1	84.0(2)	O1–Cd1–O25	89.9(1)
O1–Cd1–O4A	140.4(1)	O7–Cd2–O9B	87.1(2)
O7–Cd2–N4	137.2(2)	O9B–Cd2–N4	135.7(2)
O7–Cd2–O27	87.8(2)	O9B–Cd2–O27	90.0(2)
N4–Cd2–O27	92.5(2)	O7–Cd2–O31	85.8(2)
O9B–Cd2–O31	106.2(2)	N4–Cd2–O31	81.2(2)
O27–Cd2–O31	162.3(1)	O7–Cd2–O8B	140.9(2)
O9B–Cd2–O8B	53.8(2)	N4–Cd2–O8B	81.9(2)
O27–Cd2–O8B	92.2(2)	O31–Cd2–O8B	103.2(2)
O6–Cd2–O7	51.8(2)	O6–Cd2–O9B	138.6(2)
O6–Cd2–N4	85.8(2)	O6–Cd2–O27	85.1(2)
O6–Cd2–O31	78.1(1)	O6–Cd2–O8B	167.2(1)
O19C–Cd3–O12	135.0(2)	O19C–Cd3–O28	92.5(2)
O12–Cd3–O28	86.8(2)	O19C–Cd3–O29	95.5(2)
O12–Cd3–O29	87.7(2)	O28–Cd3–O29	172.0(2)
O19C–Cd3–N7	85.2(2)	O12–Cd3–N7	139.9(2)
O28–Cd3–N7	91.4(2)	O29–Cd3–N7	89.1(2)
O19C–Cd3–O20C	53.6(1)	O12–Cd3–O20C	81.3(1)
O28–Cd3–O20C	90.7(1)	O29–Cd3–O20C	94.2(1)
N7–Cd3–O20C	138.8(2)	O19C–Cd3–O13	169.8(1)
O12–Cd3–O13	53.8(1)	O28–Cd3–O13	82.2(1)
O29–Cd3–O13	89.9(1)	N7–Cd3–O13	86.2(2)

O20C–Cd3–O13	134.8(1)	O18–Cd4–O14	139.0(2)
O18–Cd4–O30	89.3(2)	O14–Cd4–O30	90.0(2)
O18–Cd4–N9	85.0(2)	O14–Cd4–N9	92.5(2)
O30–Cd4–N9	173.6(2)	O18–Cd4–N5	137.2(2)
O14–Cd4–N5	83.9(2)	O30–Cd4–N5	91.8(2)
N9–Cd4–N5	94.4(2)	O18–Cd4–O15	86.2(1)
O14–Cd4–O15	52.7(1)	O30–Cd4–O15	87.5(1)
N9–Cd4–O15	89.3(1)	N5–Cd4–O15	136.6(2)
O17–Cd4–O18	52.0(1)	O17–Cd4–O14	168.8(2)
O17–Cd4–O30	92.6(1)	O17–Cd4–N9	86.0(1)
O17–Cd4–N5	85.0(2)	O17–Cd4–O15	138.2(1)

4

Cd1–O5A	2.199(2)	Cd1–N1	2.312(2)
Cd1–O3	2.353(2)	Cd1–O6	2.354(2)
Cd1–O2	2.382(2)	Cd1–O7	2.385(3)
Cd1–O4A	2.779(3)		

O5A–Cd1–N1	138.80(9)	O5A–Cd1–O3	81.14(9)
N1–Cd1–O3	140.03(9)	O5A–Cd1–O6	91.7(1)
N1–Cd1–O6	85.21(9)	O3–Cd1–O6	97.2(1)
O5A–Cd1–O2	135.19(9)	N1–Cd1–O2	85.59(9)
O3–Cd1–O2	54.59(8)	O6–Cd1–O2	99.68(9)
O5A–Cd1–O7	88.7(1)	N1–Cd1–O7	81.6(1)
O3–Cd1–O7	102.4(1)	O6–Cd1–O7	160.3(1)
O2–Cd1–O7	93.9(1)	O4A–Cd1–O5A	50.57(8)
O4A–Cd1–N1	88.29(8)	O4A–Cd1–O3	131.67(8)
O4A–Cd1–O6	84.12(8)	O4A–Cd1–O2	172.49(8)
O4A–Cd1–O7	80.87(8)		

5

Cd1–O12A	2.289(5)	Cd1–O14	2.294(6)
Cd1–O4	2.320(5)	Cd1–N5	2.345(6)
Cd1–N1	2.378(7)	Cd1–O5	2.580(5)
Cd1–O11A	2.581(5)	Cd2–O7B	2.211(5)
Cd2–N8	2.306(6)	Cd2–O15	2.338(6)
Cd2–O9	2.381(5)	Cd2–O10	2.382(5)
Cd2–N9	2.427(8)	Cd2–O8B	2.741(6)

O12A–Cd1–O14	93.8(2)	O12A–Cd1–O4	81.2(2)
O14–Cd1–O4	87.0(2)	O12A–Cd1–N5	140.8(2)
O14–Cd1–N5	87.8(2)	O4–Cd1–N5	138.0(2)
O12A–Cd1–N1	90.3(2)	O14–Cd1–N1	173.3(2)
O4–Cd1–N1	98.9(2)	N5–Cd1–N1	85.7(2)
O12A–Cd1–O5	133.5(2)	O14–Cd1–O5	86.8(2)
O4–Cd1–O5	52.4(2)	N5–Cd1–O5	85.7(2)
N1–Cd1–O5	94.3(2)	O12A–Cd1–O11A	53.2(2)
O14–Cd1–O11A	90.5(2)	O4–Cd1–O11A	134.1(2)
N5–Cd1–O11A	87.6(2)	N1–Cd1–O11A	87.7(2)
O5–Cd1–O11A	172.9(2)	O7B–Cd2–N8	135.9(2)
O7B–Cd2–O15	83.9(2)	N8–Cd2–O15	80.6(2)
O7B–Cd2–O9	137.1(2)	N8–Cd2–O9	86.5(2)
O15–Cd2–O9	100.1(2)	O7B–Cd2–O10	82.4(2)
N8–Cd2–O10	140.3(2)	O15–Cd2–O10	96.7(2)
O9–Cd2–O10	54.7(2)	O7B–Cd2–N9	96.4(2)
N8–Cd2–N9	93.4(2)	O15–Cd2–N9	171.3(2)
O9–Cd2–N9	85.6(2)	O10–Cd2–N9	92.0(2)
O8B–Cd2–O7B	51.4(2)	O8B–Cd2–N8	88.4(2)
O8B–Cd2–O15	93.1(2)	O8B–Cd2–O9	164.9(2)
O8B–Cd2–O10	131.3(2)	O8B–Cd2–N9	80.5(2)

6

Cd1–O2	2.222(2)	Cd1–O3A	2.274(2)
Cd1–N1	2.348(3)	Cd1–N4B	2.353(3)
Cd1–O4C	2.369(2)	Cd1–O5C	2.395(2)
Cd1–O3	2.868(4)		
O2–Cd1–O3A	127.98(9)	O2–Cd1–N1	92.9(1)
O3A–Cd1–N1	89.5(1)	O2–Cd1–N4B	93.7(1)
O3A–Cd1–N4B	84.8(1)	N1–Cd1–N4B	173.06(9)
O2–Cd1–O4C	143.34(9)	O3A– Cd1–O4C	88.64(9)
N1–Cd1–O4C	88.67(9)	N4B–Cd1–O4C	87.36(9)
O2–Cd1–O5C	88.41(9)	O3A–Cd1–O5C	143.55(9)
N1–Cd1–O5C	90.8(1)	N4B–Cd1–O5C	91.6(1)
O4C–Cd1–O5C	54.93(8)	O3–Cd1–O2	48.50(9)
O3–Cd1–O3A	79.5(1)	O3–Cd1–N1	95.4(1)
O3–Cd1–N4B	87.3(1)	O3–Cd1–O4C	167.40(9)
O3–Cd1–O5C	136.66(9)		

Symmetry codes: A = $x - 1, y, z$ for **1**; A = $x, y, z + 1$; B = $-x + 1/2, -y + 3/2, -z + 3/2$ for **2**; A = $-x - 1/2, y + 1/2, -z + 1$; B = $-x + 1/2, y + 1/2, -z$; C = $x, y - 1, z$ for **3**; A = $-x + 1/2, y - 1/2, -z + 3/2$ for **4**; A = $x, y - 1, z$; B = $x, y + 1, z + 1$ for **5**; A = $-x + 1, -y + 1, -z + 1$; B = $-x + 2, -y + 1, -z + 1$; C = $x + 1, y, z$ for **6**.

Table S2 Important hydrogen-bonding geometries (Å, °) for complexes **1**, **3**, **4**, and **5**

D–H···A	D···A	H···A	D–H···A	Symmetry code
1				
O11–H11A···N3	2.983(5)	2.14	172	$-x + 1, -y, -z + 1$
O11–H11B···N6	2.951(5)	2.17	153	$-x + 1, -y + 1, -z$
O12–H12A···O4	2.938(4)	2.26	136	$x - 1, y, z$
O12–H12B···O14	2.690(8)	2.03	133	
3				
O25–H25A···N8	2.967(6)	2.13	167	$-x, y, -z + 1$
O25–H25B···O13	2.770(5)	1.96	159	$-x, y, -z + 1$
O26–H26A···O33	2.695(6)	1.97	143	$x - 1/2, y - 1/2, z$
O27–H27A···O17	2.837(6)	2.08	148	$-x + 1/2, y - 1/2, -z$
O27–H27B···N6	3.003(7)	2.19	161	$-x + 1/2, y - 1/2, -z$
O28–H28A···O32	2.719(8)	1.92	157	
O28–H28B···O4	2.732(6)	2.09	132	$x + 1/2, y + 1/2, z$
O29–H29A···O6	2.723(5)	1.88	172	
O29–H29B···N3	2.957(6)	2.12	170	
O30–H30A···O1	2.781(5)	1.94	174	$x + 1/2, y + 1/2, z$
O30–H30B···N2	2.859(7)	2.04	161	$x + 1/2, y + 1/2, z$
4				
O6–H6A···O4	2.705(3)	1.86	174	$-x + 1/2, -y + 1/2, -z + 1$
O6–H6B···N2	3.061(4)	2.23	166	$x, -y, z - 1/2$
O7–H7A···O3	2.686(4)	1.86	162	$x, -y, z + 1/2$
5				

O6–H6···O17	2.67(1)	1.85	174	$-x + 1, -y + 1, -z$
O13–H13···O20	2.71(1)	1.89	174	
O14–H14A···O10	2.855(9)	2.24	129	$-x + 1, -y + 1, -z + 1$
O15–H15A···O5	2.813(9)	2.01	158	$-x + 1, -y + 1, -z + 1$
O15–H15B···O19	2.83(1)	2.13	139	$-x + 1, -y + 1, -z + 1$
O16–H16A···N6	2.870(9)	2.03	170	$-x + 1, -y, -z + 1$
O16–H16B···O11	2.820(8)	1.97	173	$-x + 1, -y + 1, -z + 1$