Electronic Supplementary Information (ESI) for

Multifarious Zn^{II} and Cd^{II} coordination frameworks constructed by a versatile *trans*-1-(2-pyridyl)-2-(4-pyridyl)ethylene tecton and various benzenedicarboxyl ligands

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Experimental details

{[Zn(bpe)$_2$(ip)](H$_2$O)$_2$}$_n$ (1). Reactants: H_2ip (16.6 mg, 0.1 mmol), bpe (18.4 mg, 0.1 mmol), and $Zn(NO_3)_2 \cdot 6H_2O$ (29.8 mg, 0.1 mmol). Pale-yellow prism crystals were obtained after two days. Yield: 17.3 mg (55%, based on bpe). Anal. Calcd for $C_{32}H_{28}N_4O_6Zn$ (**1**): C, 61.01; H, 4.48; N, 8.89%. Found: C, 61.17; H, 4.39; N, 9.03%. IR (cm^{-1}): 3423b, 3063w, 1611vs, 1563s, 1391vs, 1221m, 1155m, 1073w, 1018w, 969m, 821m, 740m, 665w, 550w.

{[Cd$_2$(bpe)$_2$(ip)$_2$(CH$_3$OH)(H$_2$O)](H$_2$O)$_4$}$_n$ (2). Reactants: H_2ip (16.6 mg, 0.1 mmol), bpe (18.4 mg, 0.1 mmol), and $Cd(NO_3)_2 \cdot 4H_2O$ (30.8 mg, 0.1 mmol). Yellow block crystals were obtained after one week. Yield: 46% (23.9 mg). Anal. Calcd for $C_{41}H_{42}N_4O_{14}Cd_2$ (**2**): C, 47.37; H, 4.07; N, 5.39%. Found: 47.25; H, 3.95; N, 5.51%. IR (cm^{-1}): 3422b, 2922w, 1607vs, 1554vs, 1474w, 1432s, 1385vs, 1223w, 1158w, 1102w, 1073w, 1013w, 967w, 816m, 743m, 719m, 542w.

{[Zn(bpe)$_2$(hip)](H$_2$O)$_{1.25}$}$_n$ (3). Reactants: H_2hip (18.2 mg, 0.1 mmol), bpe (18.4 mg, 0.1 mmol), and $Zn(NO_3)_2 \cdot 6H_2O$ (29.8 mg, 0.1 mmol). Yellow block crystals were obtained after five days. Yield: 15.6 mg (49%, based on bpe). Anal. Calcd for $C_{32}H_{26.5}N_4O_{6.25}Zn$ (**3**): C, 60.77; H, 4.22; N, 8.86%. Found: C, 60.38; H, 4.51; N, 8.57%. IR (cm^{-1}): 3417b, 1617vs, 1567vs, 1494w, 1399vs, 1285s, 1216m, 1152w, 1105w, 972m, 910w, 780m, 724w, 627w, 544w, 457w.

{[Cd$_2$(bpe)$_2$(hip)$_2$(CH$_3$OH)(H$_2$O)](H$_2$O)$_4$}$_n$ (4). Reactants: H_2hip (18.2 mg, 0.1 mmol), bpe (18.4 mg, 0.1 mmol), and $Cd(NO_3)_2 \cdot 4H_2O$ (30.8 mg, 0.1 mmol). Colorless block crystals were obtained after three days. Yield: 20.9 mg (39%). Anal. Calcd for $C_{41}H_{42}N_4O_{16}Cd_2$ (**4**): C, 45.95; H, 3.95; N, 5.23%. Found: C, 46.08; H, 4.02; N, 5.01%. IR (cm^{-1}): 3429b, 1609s, 1565vs, 1479w, 1428s, 1390vs, 1306w, 1284w, 1220w. 1155w, 1095w, 1007m, 967w, 910w, 877w, 813w, 786s, 722m, 690w, 662w, 562w, 540w, 489w.

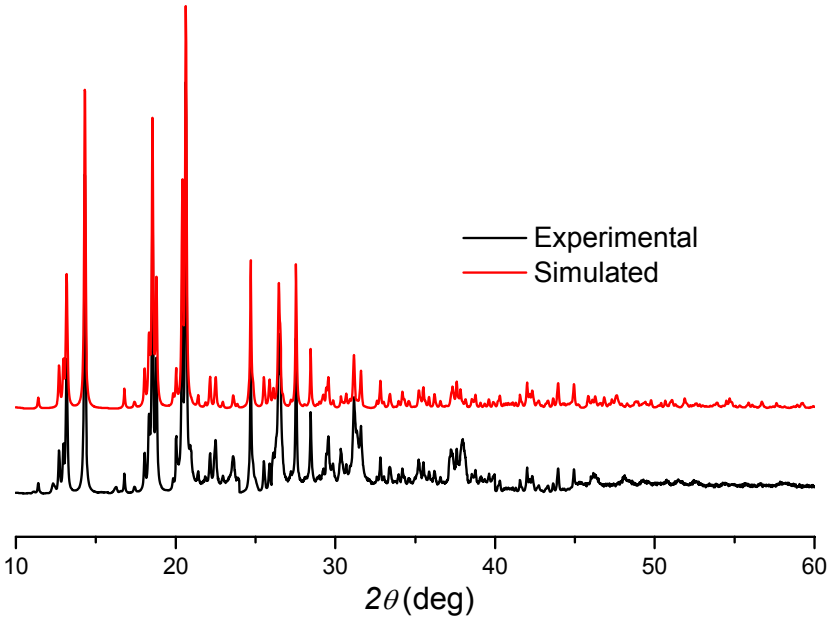
{[Zn$_2$(bpe)$_2$(tp)$_2$](H$_2$O)}$_n$ (5). Reactants: H_2tp (16.6 mg, 0.1 mmol), bpe (18.4 mg, 0.1 mmol), and $Zn(NO_3)_2 \cdot 6H_2O$ (29.8 mg, 0.1 mmol). Yellow block crystals were obtained after

one week. Yield: 25.2 mg (60%). Anal. Calcd for $C_{40}H_{30}N_4O_9Zn_2$ (**5**): C, 57.10; H, 3.59; N, 6.66%. Found: C, 57.73; H, 3.65; N, 6.39%. IR (cm^{-1}): 3419b, 1609vs, 1503m, 1389vs, 1221w, 1146w, 1091w, 1025w, 972w, 886w, 827s, 748s, 544m.

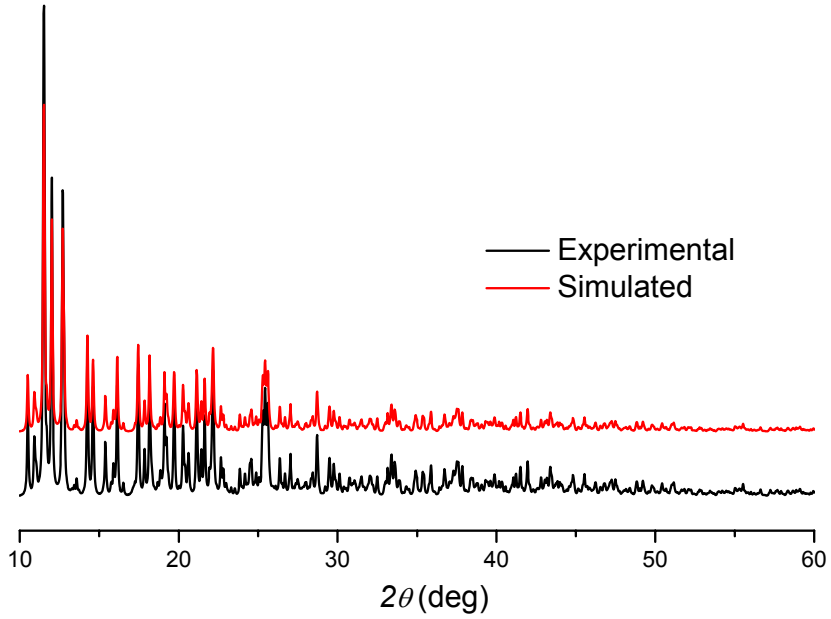
{[Cd(bpe)(tp)(H_2O)](H_2O)}$_n$ (6). Reactants: H_2tp (16.6 mg, 0.1 mmol), bpe (18.4 mg, 0.1 mmol), and $Cd(NO_3)_2{\cdot}4H_2O$ (30.8 mg, 0.1 mmol). Colorless block crystals were obtained after one week. Yield: 20.3 mg (41%). Anal. Calcd for $C_{20}H_{18}N_2O_6Cd$ (**6**): C, 48.55; H, 3.67; N, 5.66%. Found: C, 48.37; H, 3.79; N, 5.42%. IR (cm^{-1}): 3446b, 1650w, 1608m, 1566vs, 1499w, 1476w, 1429w, 1400s, 1218w, 1157w, 1090w, 1007w, 966w, 882w, 817m, 743m, 669w, 541w, 505w.

[Zn(bpe)$_2$(tbta)(H_2O)]$_n$ (7). Reactants: H_2tbta (48.2 mg, 0.1 mmol), bpe (18.4 mg, 0.1 mmol), and $Zn(NO_3)_2{\cdot}6H_2O$ (29.8 mg, 0.1 mmol). Orange block crystals were obtained after ten days. Yield: 21.8 mg (47%, based on bpe). Anal. Calcd for $C_{32}H_{22}N_4O_5Br_4Zn$ (**7**): C, 41.44; H, 2.39; N, 6.04%. Found: C, 41.28; H, 2.41; N, 6.19%. IR (cm^{-1}): 3418b, 1643vs, 1601vs, 1419s, 1317vs, 1083w, 1012w, 975w, 888w, 823m, 766w, 693w, 577m, 539m.

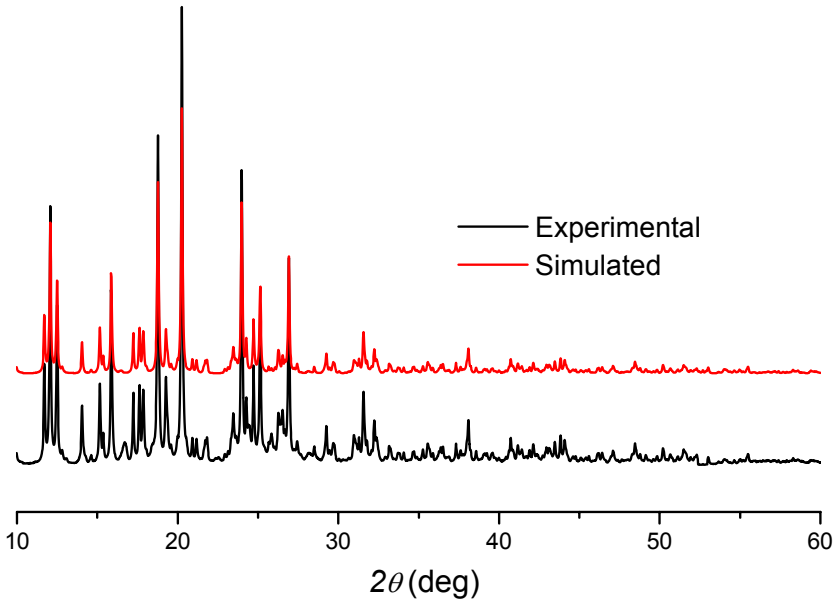
[Cd(Hbpe)$_2$(tbta)$_2$(H_2O)$_2$](H_2tbta) (8). Reactants: H_2tbta (48.2 mg, 0.1 mmol), bpe (18.4 mg, 0.1 mmol), and $Cd(NO_3)_2{\cdot}4H_2O$ (30.8 mg, 0.1 mmol). Colorless block crystals were obtained after one week. Yield: 27.4 mg (42%, based on H_2tbta). Anal. Calcd for $C_{48}H_{28}N_4O_{14}Br_{12}Cd$ (**8**): C, 29.47; H, 1.44; N, 2.86%. Found: C, 29.32; H, 1.31; N, 3.01%. IR (cm^{-1}): 3442b, 3075m, 2465m, 1961m, 1706s, 1628vs, 1500m, 1375w, 1325s, 1280s, 1189m, 1088m, 1023m, 969s, 873w, 811s, 692w, 652w, 555m.


Experimental
Simulated
10
20
30
40
50
60
2θ(deg)

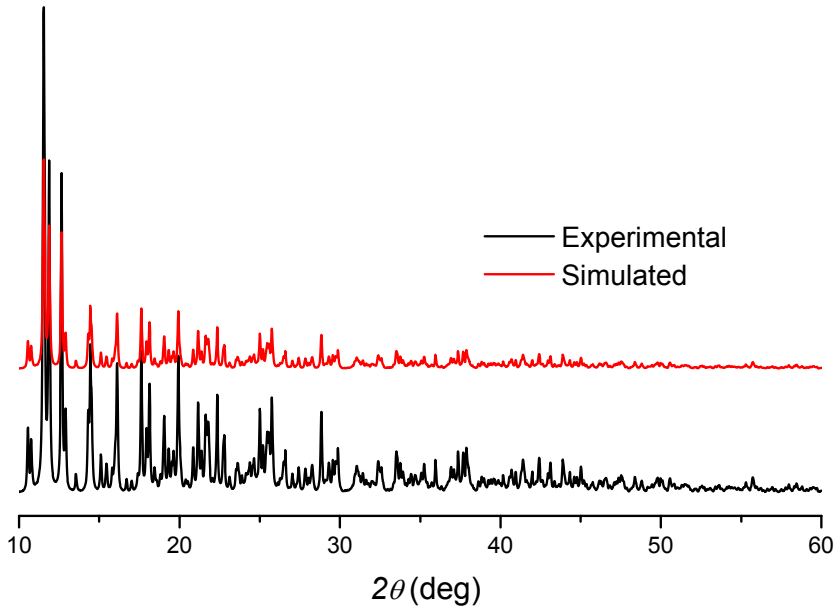
(a)


Experimental
Simulated
10
20
30
40
50
60
2θ(deg)

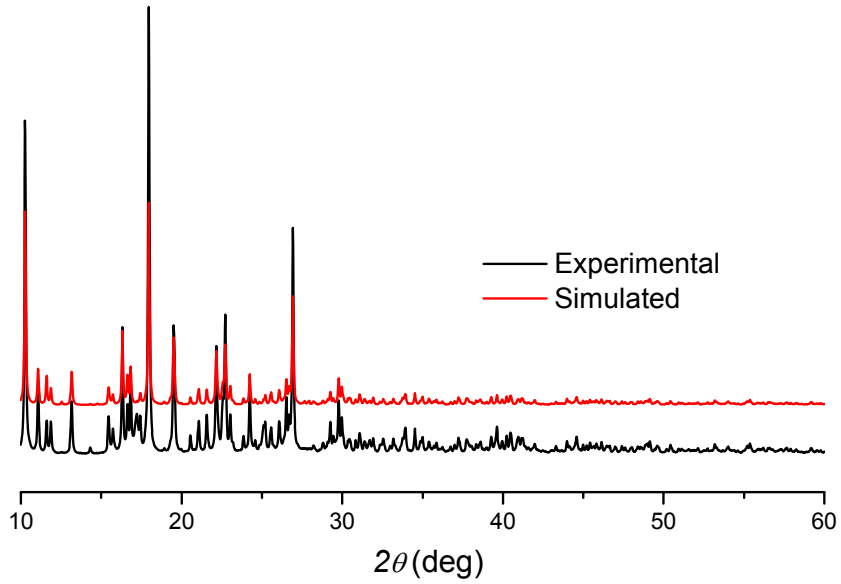
(b)


Experimental
Simulated
10
20
30
40
50
60
2θ (deg)

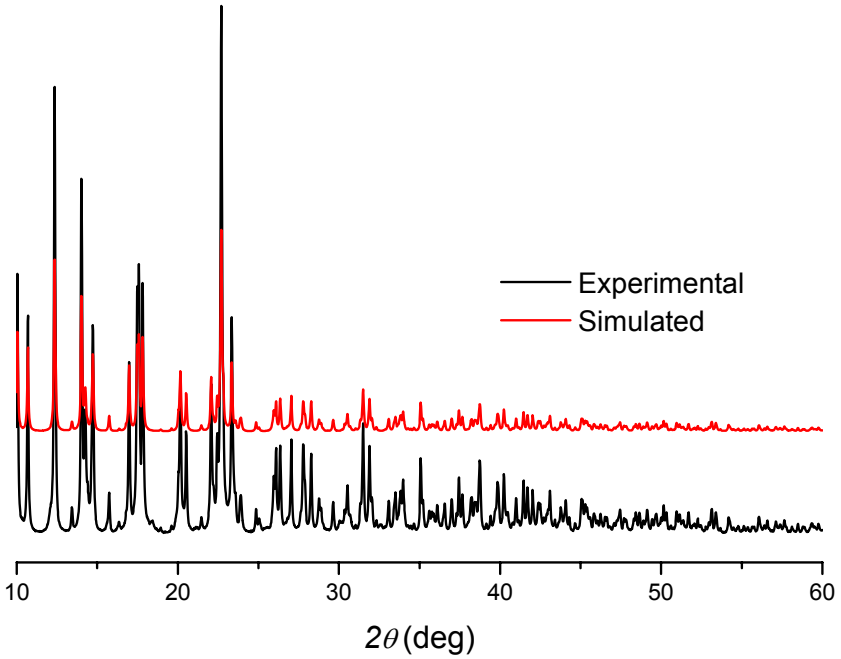
(c)


Experimental
Simulated
10
20
30
40
50
60
2θ (deg)

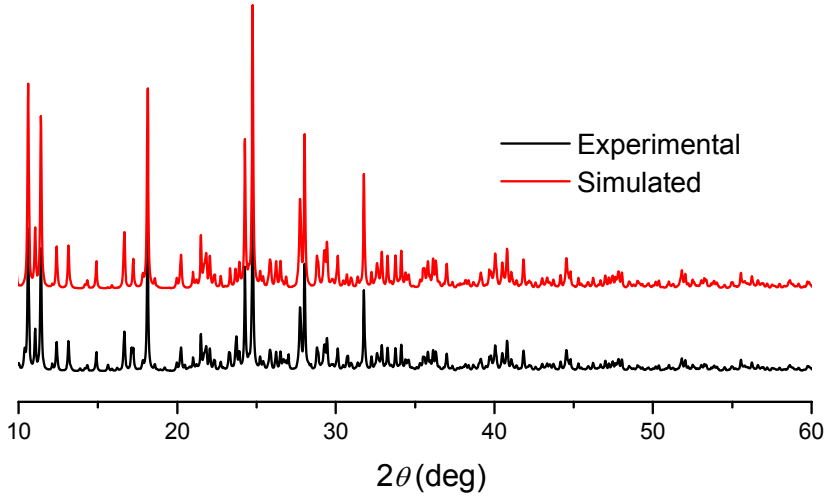
(d)


Experimental
Simulated
10
20
30
40
50
60
2θ (deg)

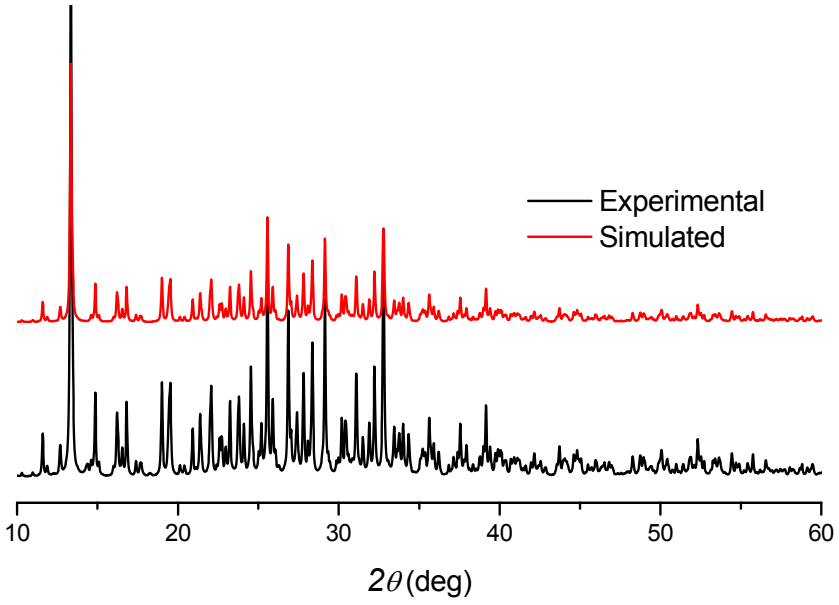
(e)


Experimental
Simulated
10
20
30
40
50
60
2θ (deg)

(f)



(g)



(h)

Fig. S1 Powder X-ray diffraction (PXRD) patterns for complexes **1**–**8** (**a**–**h**).

Table S1 Selective bond lengths (Å) and angles (°) for complexes **1**–**8**

1

Zn1–O1	2.420(2)	Zn1–O2	2.112(2)
Zn1–O3A	2.037(2)	Zn1–O4B	2.047(2)
Zn1–N1	2.150(3)	Zn1–N3	2.164(2)
O1–Zn1–O2	57.38(7)	O1–Zn1–O3A	148.49(7)
O1–Zn1–O4B	97.35(7)	O1–Zn1–N1	94.9(2)
O1–Zn1–N3	83.3(1)	O2–Zn1–O3A	91.99(7)
O2–Zn1–O4B	154.65(8)	O2–Zn1–N1	94.7(2)
O2–Zn1–N3	90.1(1)	O3A–Zn1–O4B	112.69(7)
O3A–Zn1–N1	94.9(2)	O3A–Zn1–N3	90.2(1)
O4B–Zn1–N1	89.1(2)	O4B–Zn1–N3	84.4(1)
N1–Zn1–N3	173.0(2)		

2

Cd1–O5	2.436(3)	Cd1–O6	2.316(3)
Cd1–O8B	2.240(3)	Cd1–O9	2.386(4)
Cd1–N4C	2.311(4)	Cd1–N2	2.406(4)
Cd2–O10	2.292(3)	Cd2–O1	2.471(3)
Cd2–O2	2.349(3)	Cd2–O3A	2.442(3)
Cd2–O4A	2.412(3)	Cd2–N1	2.350(4)
Cd2–N3	2.344(4)		
O5–Cd1–O6	55.1(1)	O5–Cd1–O8B	155.9(1)
O5–Cd1–O9	80.6(1)	O5–Cd1–N2	102.2(1)
O5–Cd1–N4C	89.2(1)	O6–Cd1–O8B	104.8(1)
O6–Cd1–O9	92.9(1)	O6–Cd1–N2	87.7(1)
O6–Cd1–N4C	144.0(1)	O8B–Cd1–O9	88.1(1)
O8B–Cd1–N2	88.8(1)	O8B–Cd1–N4C	110.8(1)
O9–Cd1–N2	176.9(1)	O9–Cd1–N4C	83.8(1)
N2–Cd1–N4C	97.6(1)	O1–Cd2–O2	54.3(1)
O1–Cd2–O3A	88.4(1)	O1–Cd2–O4A	142.4(1)
O1–Cd2–O10	135.4(1)	O1–Cd2–N1	86.7(1)

O1–Cd2–N3	87.1(1)	O2–Cd2–O3A	142.5(1)
O2–Cd2–O4A	163.3(1)	O2–Cd2–O10	81.1(1)
O2–Cd2–N1	92.2(1)	O2–Cd2–N3	98.5(1)
O3A–Cd2–O4A	54.0(1)	O3A–Cd2–O10	136.1(1)
O3A–Cd2–N1	80.7(1)	O3A–Cd2–N3	81.5(1)
O4A–Cd2–O10	82.2(1)	O4A–Cd2–N1	88.4(1)
O4A–Cd2–N3	85.8(1)	O10–Cd2–N1	96.0(1)
O10–Cd2–N3	100.8(1)	N1–Cd2–N3	161.3(1)

3

Zn1–O4A	1.973(3)	Zn1–O1	1.985(3)
Zn1–O2B	1.990(3)	Zn1–N3	2.09(1)
Zn1–N1	2.212(8)		

O4A–Zn1–O1	99.2(1)	O4A–Zn1–O2B	135.2(1)
O1–Zn1–O2B	125.0(1)	O4A–Zn1–N3	91.8(5)
O1–Zn1–N3	93.8(5)	O2B–Zn1–N3	92.1(5)
O4A–Zn1–N1	87.6(3)	O1–Zn1–N1	90.1(4)
O2B–Zn1–N1	85.7(3)	N3–Zn1–N1	176.2(6)

4

Cd1–O4A	2.231(2)	Cd1–N3	2.302(2)
Cd1–O2	2.343(2)	Cd1–O1	2.362(2)
Cd1–O11	2.405(3)	Cd1–N1	2.409(2)
Cd2–O9B	2.505(2)	Cd2–O12	2.310(2)
Cd2–O8B	2.326(2)	Cd2–N4C	2.350(2)
Cd2–N2	2.357(2)	Cd2–O7	2.400(2)
Cd2–O6	2.436(2)		

O4A–Cd1–N3	112.04(8)	O4A–Cd1–O2	152.77(8)
N3–Cd1–O2	92.20(8)	O4A–Cd1–O1	100.07(8)
N3–Cd1–O1	147.62(8)	O2–Cd1–O1	55.55(8)
O4A–Cd1–O11	90.79(9)	N3–Cd1–O11	83.4(1)
O2–Cd1–O11	79.46(9)	O1–Cd1–O11	92.3(1)
O4A–Cd1–N1	89.83(8)	N3–Cd1–N1	98.63(9)

O2–Cd1–N1	98.94(8)	O1–Cd1–N1	85.19(9)
O11–Cd1–N1	177.5(1)	O8B–Cd2–N4C	97.57(8)
O12–Cd2–O8B	81.36(8)	O12–Cd2–N4C	99.55(9)
O12–Cd2–N2	95.12(9)	O8B–Cd2–N2	92.25(9)
N4C–Cd2–N2	163.40(9)	O12–Cd2–O7	83.23(8)
O8B–Cd2–O7	164.50(7)	N4C–Cd2–O7	86.51(8)
N2–Cd2–O7	87.56(8)	O12–Cd2–O6	137.25(8)
O8B–Cd2–O6	141.13(7)	N4C–Cd2–O6	82.35(8)
N2–Cd2–O6	81.61(8)	O7–Cd2–O6	54.13(6)
O12–Cd2–O9B	135.23(7)	O8B–Cd2–O9B	53.94(7)
N4C–Cd2–O9B	89.66(8)	N2–Cd2–O9B	85.33(8)
O7–Cd2–O9B	141.34(6)	O6–Cd2–O9B	87.24(6)

5

Zn1–O1	1.933(2)	Zn1–O5	1.959(2)
Zn1–O8A	1.971(2)	Zn1–N3	2.020(3)
Zn2–O4B	1.948(3)	Zn2–O7A	1.962(2)
Zn2–O6	1.981(2)	Zn2–N1	2.017(3)
O1–Zn1–O5	110.0(1)	O1–Zn1–O8A	104.0(1)
O5–Zn1–O8A	115.3(1)	O1–Zn1–N3	122.7(3)
O5–Zn1–N3	106.0(2)	O8A–Zn1–N3	98.8(2)
O4B–Zn2–O7A	114.5(1)	O4B–Zn2–O6	104.1(1)
O7A–Zn2–O6	112.8(1)	O4B–Zn2–N1	124.3(1)
O7A–Zn2–N1	101.0(1)	O6–Zn2–N1	99.3(1)

6

Cd1–O5	2.316(4)	Cd1–O3A	2.354(3)
Cd1–N2B	2.361(4)	Cd1–N1	2.384(4)
Cd1–O2	2.386(3)	Cd1–O1	2.482(4)
Cd1–O4A	2.489(4)		
O5–Cd1–O3A	88.0(1)	O5–Cd1–N2B	82.5(1)
O3A–Cd1–N2B	148.7(1)	O5–Cd1–N1	167.1(1)
O3A–Cd1–N1	87.0(1)	N2B–Cd1–N1	95.8(1)

O5–Cd1–O2	83.1(1)	O3A–Cd1–O2	86.9(1)
N2B–Cd1–O2	121.2(1)	N1–Cd1–O2	108.4(1)
O5–Cd1–O1	108.3(1)	O3A–Cd1–O1	132.6(1)
N2B–Cd1–O1	78.7(1)	N1–Cd1–O1	83.7(1)
O2–Cd1–O1	53.(1)	O5–Cd1–O4A	87.3(1)
O3A–Cd1–O4A	54.0(1)	N2B–Cd1–O4A	95.7(1)
N1–Cd1–O4A	80.1(1)	O2–Cd1–O4A	140.0(1)
O1–Cd1–O4A	162.3(1)		

7

Zn1–O1	2.006(3)	Zn1–O5	2.030(3)
Zn1–O3A	2.074(3)	Zn1–N1	2.187(4)
Zn1–N3	2.197(4)		
O1–Zn1–O5	121.1(1)	O1–Zn1–O3A	93.7(1)
O5–Zn1–O3A	145.3(1)	O1–Zn1–N1	96.4(1)
O5–Zn1–N1	87.2(1)	O3A–Zn1–N1	89.0(1)
O1–Zn1–N3	93.0(1)	O5–Zn1–N3	88.9(1)
O3A–Zn1–N3	89.3(1)	N1–Zn1–N3	170.6(1)

8

Cd1–O2	2.283(3)	Cd1–O7	2.325(4)
Cd1–N1	2.353(4)		
O2–Cd1–O7	91.5(1)	O2–Cd1–N1	85.5(2)
O7–Cd1–N1	87.8(2)		

Symmetry codes: A = $-x + 1, -y + 1, -z + 1$; B = $x - 1, y, z$ for **1**; A = $-x + 1, y + 1/2, -z + 3/2$; B = $-x, y + 1/2, -z + 1/2$; C = $x - 1, -y + 1/2, z - 1/2$ for **2**; A = $-x, y + 1/2, -z + 1/2$; B = $-x, -y + 2, -z + 1$ for **3**; A = $-x + 2, y + 1/2, -z + 5/2$; B = $-x + 1, y - 1/2, -z + 3/2$; C = $x - 1, -y + 3/2, z - 1/2$ for **4**; A = $x + 1, y, z$; B = $x, y - 1, z$ for **5**; A = $x + 1/2, -y + 1/2, z + 1/2$; B = $-x + 1/2, y + 1/2, -z + 3/2$ for **6**; A = $x - 1/2, -y + 1/2, z + 1/2$ for **7**.

Table S2 Possible hydrogen-bonding geometries (Å, °)

D–H···A	D···A	H···A	D–H···A	Symmetry code
1				
O6–H6A···O5	2.659(6)	2.06	127	$-x, -y + 1, -z + 1$
O6–H6B···N4	2.884(7)	2.08	156	
2				
O10–H10A···O4	2.732(4)	1.90	167	$x, -y - 1/2, z + 1/2$
O10–H10B···O13	2.804(8)	1.99	160	$x, y - 1, z$
O11–H11B···O13	2.78(1)	1.99	156	
O12–H12A···O1	2.752(5)	1.92	168	$-x + 1, -y + 1, -z + 1$
3				
O5–H5B···O3	2.669(5)	1.86	176	$-x, y - 1/2, -z + 1/2$
4				
O5–H5···O14	2.679(4)	1.86	177	$x, y, z + 1$
O10–H10···O13	2.698(3)	1.88	176	$x, -y + 3/2, z - 1/2$
O11–H11A···O3	2.664(4)	1.88	152	$-x + 2, y + 1/2, -z + 5/2$
O12–H12A···O7	2.718(3)	1.87	172	$-x + 1, -y + 1, -z + 1$
O12–H12B···O15	2.804(6)	1.98	162	$x, -y + 1/2, z + 1/2$
O13–H13A···O9	2.785(3)	1.95	169	$-x + 1, y - 1/2, -z + 3/2$
O13–H13B···O5	2.843(3)	2.03	161	
O14–H14A···O15	2.780(7)	1.98	156	
O14–H14B···O6	2.820(4)	1.97	175	$-x + 1, -y + 1, -z + 1$
6				
O5–H5A···O6	2.647(8)	1.80	171	
O5–H5B···O2	2.692(5)	1.96	144	$-x + 1/2, -y + 1/2, -z + 2$

7

O5–H5A···O4	2.664(4)	1.82	170	$-x + 3/2, y - 1/2, -z + 3/2$
O5–H5B···N2	2.782(5)	1.97	159	$-x + 2, -y, -z + 2$

8

O7–H7A···O4	2.745(5)	1.93	160	$x + 1/2, -y + 1/2, z + 1/2$
O5–H5A···O3	2.454(5)	1.65	166	$x + 1/2, -y + 1/2, z + 1/2$
N2–H2A···O6	2.717(6)	1.88	165	$-x + 1/2, y - 1/2, -z + 3/2$
O7–H7B···O1	2.714(6)	1.98	144	