Supplementary materials

Coordination Polymers Constructed from Semi-rigid *N,N'*-Bis(3-pyridyl)terephthalamide and Dicarboxylic Acids: Effect of Ligand Isomerism, Flexibility and Identity

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Figure S1. The PXRD patterns of complex **1**.

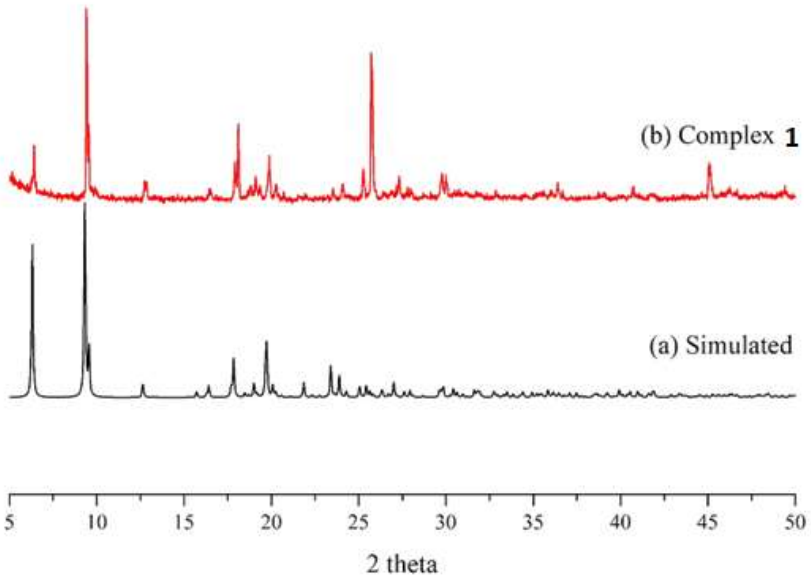

Figure S2. The PXRD patterns of complex **3**.

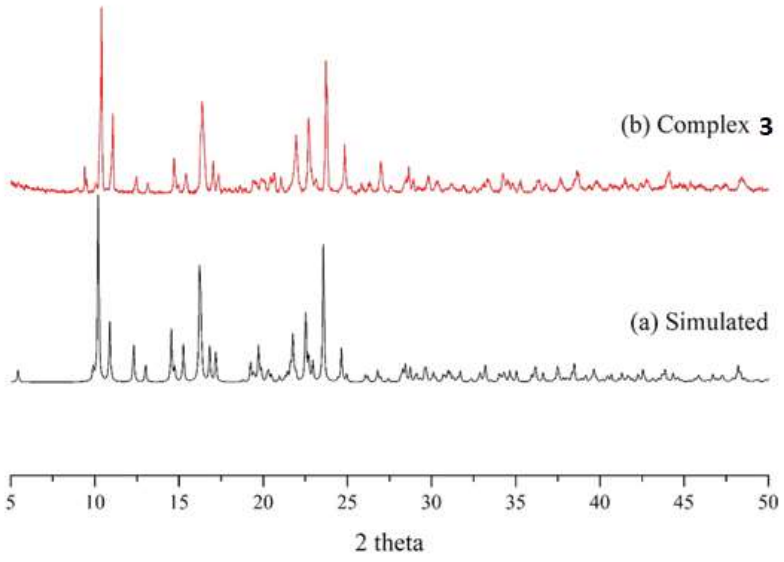

Figure S3. The PXRD patterns of complex **4**.

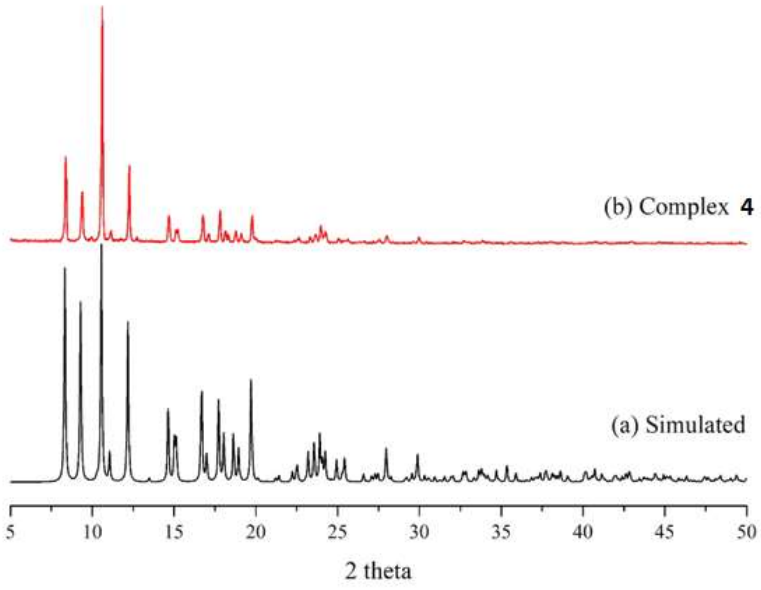

Figure S4. TGA curve of complex **1**.

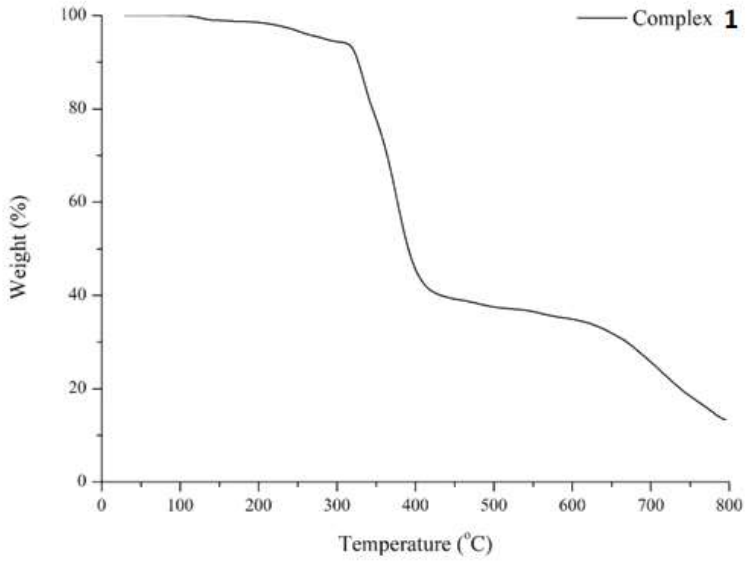

Figure S5. TGA curve of complex **3**.

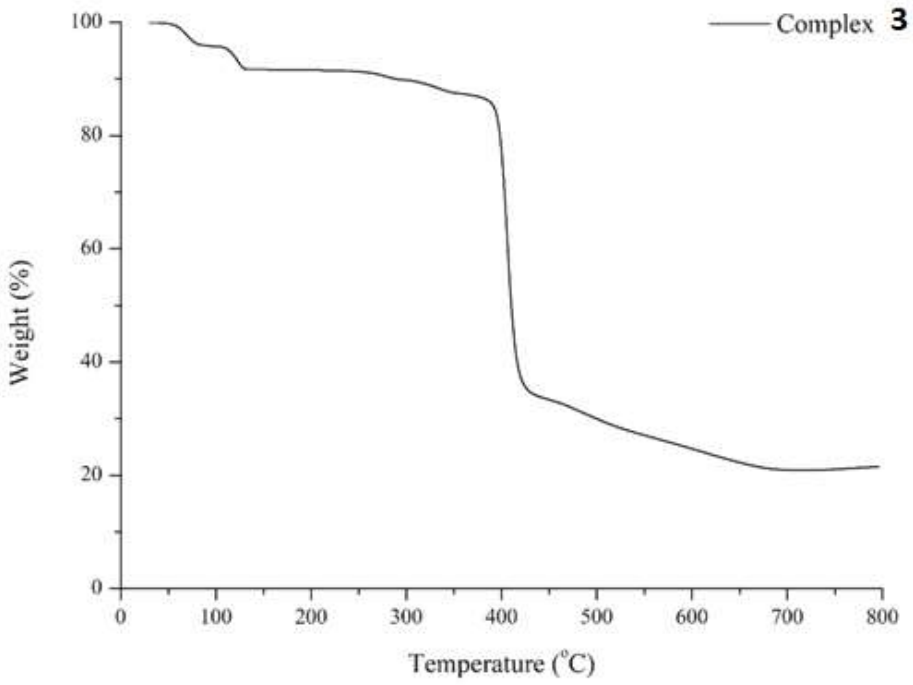

Figure S6. TGA curve of complex **4**.

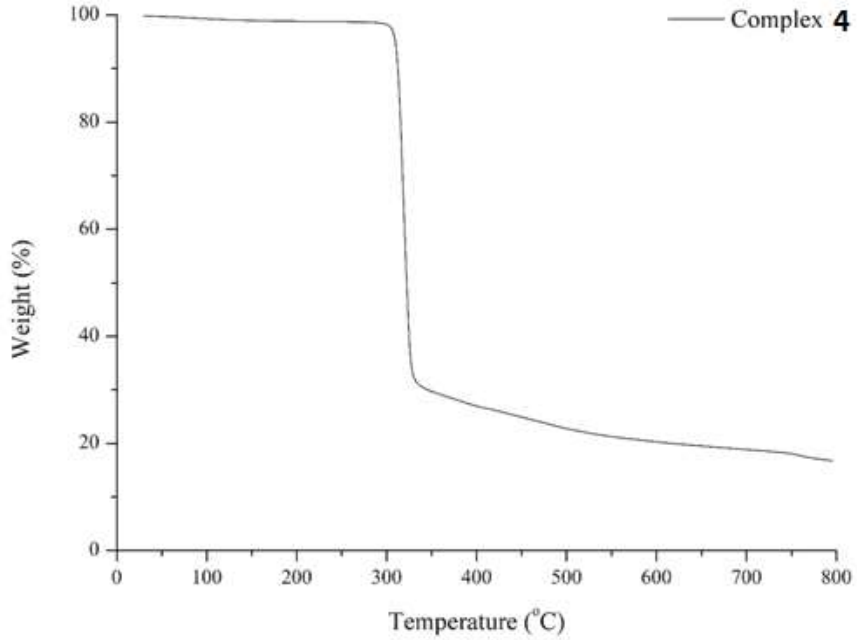

Figure S7. The photoluminescence spectra of **L**.

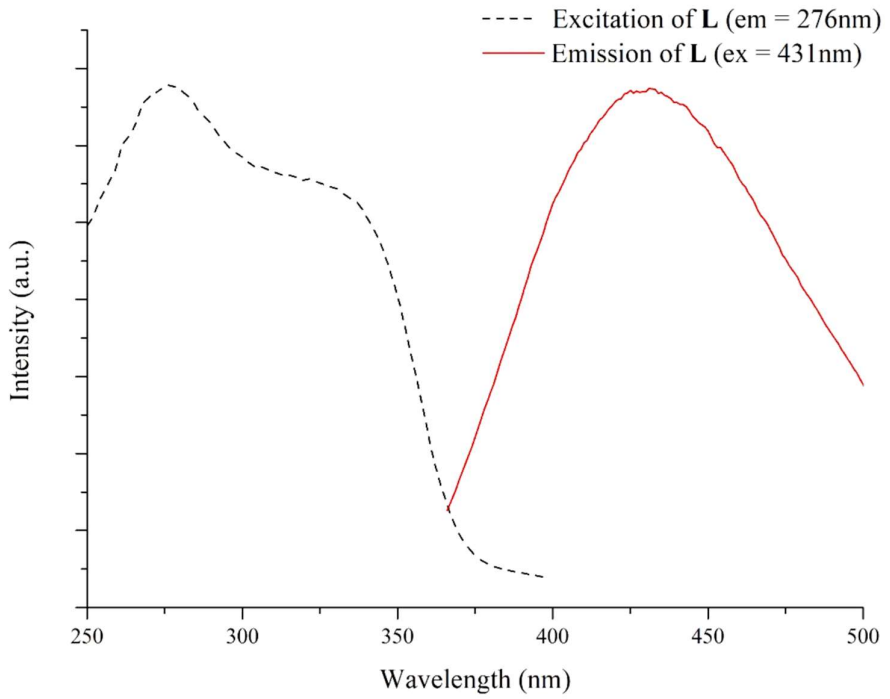

Figure S8. The photoluminescence spectra of 1,2-H_2BDC.

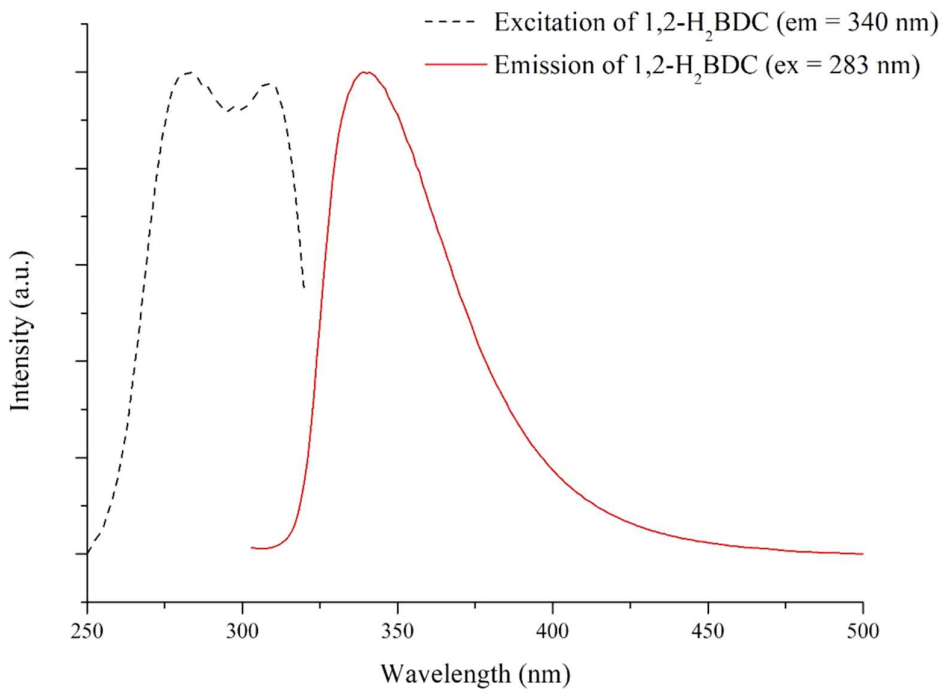

Figure S9. The photoluminescence spectra of 1,4-H_2BDC.

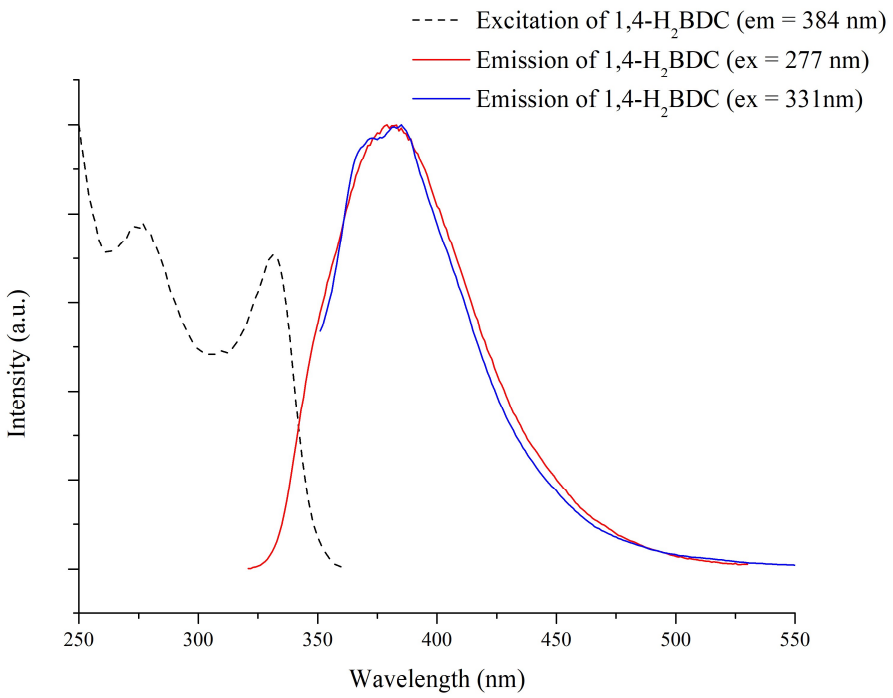

Figure S10. The photoluminescence spectra of complex **1**.

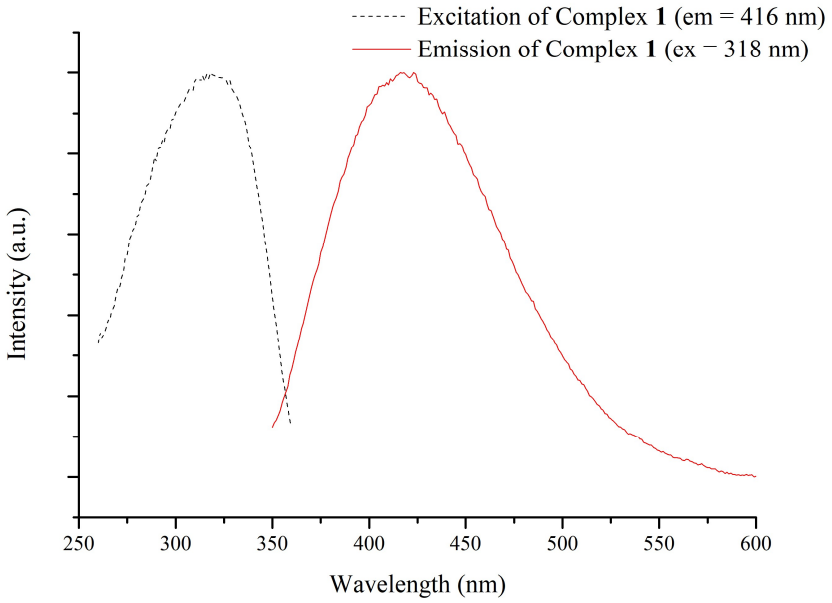

Figure S11. The photoluminescence spectra of complex **3**.

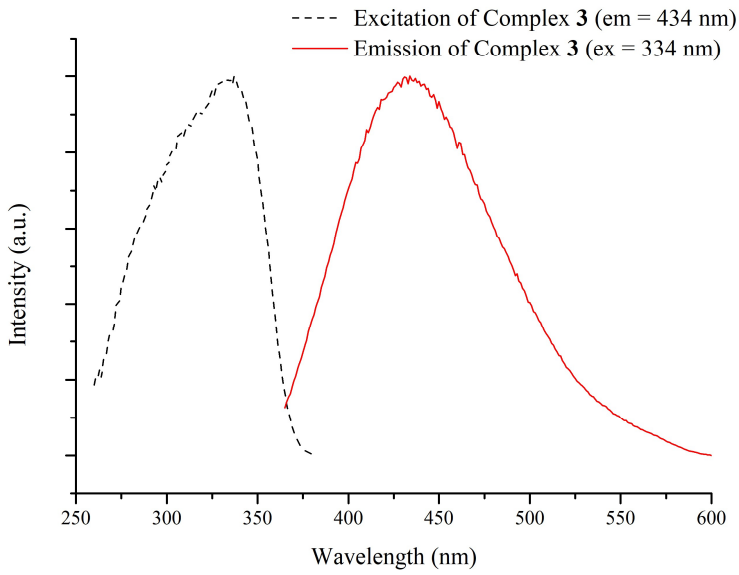

Table S1. Crystal data and structure refinement for **2a**.

Identification code	12452_0m	
Empirical formula	C35 H37 Cd N6 O13	
Formula weight	862.10	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.27390(10) Å	α= 109.9067(7)°.
	b = 12.8047(2) Å	β= 97.2783(7)°.
	c = 15.8305(2) Å	γ = 108.3033(8)°.
Volume	1794.27(4) $Å^3$	
Z	2	
Density (calculated)	1.596 Mg/m^3	
Absorption coefficient	0.685 mm^{-1}	
F(000)	882	
Crystal size	0.200 x 0.100 x 0.100 mm^3	
Theta range for data collection	1.417 to 25.999°.	
Index ranges	-12<=h<=12, -15<=k<=15, -19<=l<=19	
Reflections collected	29038	
Independent reflections	7053 [R(int) = 0.0598]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7053 / 488 / 378	
Goodness-of-fit on F^2	1.073	
Final R indices [I>2sigma(I)]	R1 = 0.1073, wR2 = 0.3116	
R indices (all data)	R1 = 0.1474, wR2 = 0.3476	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.205 and -1.557 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cd	9508(1)	9487(1)	6709(1)	33(1)
O(1)	6692(9)	3951(6)	7450(6)	30(2)
O(2)	1437(8)	4786(7)	10003(6)	31(2)
O(3)	12430(7)	15308(6)	6362(5)	23(2)
O(4)	7673(6)	8803(5)	5492(4)	8(1)
O(5)	7455(6)	9490(5)	6915(4)	12(1)
O(6)	2872(8)	10073(7)	7373(5)	25(2)
O(7)	1086(6)	9321(5)	6102(4)	10(1)
O(8)	10651(6)	10237(5)	8092(4)	11(1)
O(9)	6647(9)	9584(7)	8651(6)	34(2)
O(10)	14931(9)	17186(8)	7661(7)	42(2)
O(11)	5220(40)	11200(30)	8860(30)	31(2)
O(11')	5190(40)	11050(30)	8860(30)	32(2)
O(12)	3340(9)	1563(7)	9998(6)	34(2)
O(13)	7316(9)	2851(7)	8626(6)	35(2)
N(1)	8911(7)	7624(6)	6634(5)	8(1)
N(2)	6574(7)	5720(6)	7517(5)	7(1)
N(3)	1516(9)	2989(7)	9896(6)	18(2)
N(4)	-543(9)	1251(8)	11001(6)	22(2)
N(5)	10073(7)	11326(6)	6794(5)	7(1)
N(6)	12231(7)	13361(6)	5912(5)	7(1)
C(1)	9636(9)	6942(8)	6249(6)	14(1)
C(2)	9428(10)	5844(8)	6282(7)	18(1)
C(3)	8420(10)	5392(8)	6699(7)	17(1)
C(4)	7639(9)	6061(8)	7088(6)	13(1)
C(5)	7945(9)	7185(8)	7030(6)	12(1)
C(6)	6171(10)	4693(8)	7686(6)	14(1)
C(7)	5043(9)	4549(8)	8202(6)	13(1)
C(8)	4255(10)	3373(8)	8097(6)	14(1)
C(9)	3264(10)	3185(8)	8594(6)	15(1)
C(10)	3014(10)	4144(8)	9194(6)	14(1)
C(11)	3793(10)	5307(8)	9289(6)	15(1)
C(12)	4794(10)	5501(8)	8804(6)	14(1)

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(13)	1927(10)	4006(8)	9732(6)	15(1)
C(14)	480(10)	2655(9)	10365(7)	18(1)
C(15)	-436(11)	3234(9)	10610(7)	20(1)
C(16)	-1417(11)	2778(9)	11058(7)	23(2)
C(17)	-1436(11)	1801(9)	11246(7)	22(2)
C(18)	395(11)	1673(9)	10566(7)	20(1)
C(19)	9585(9)	12047(7)	7395(6)	9(1)
C(20)	9945(9)	13249(8)	7537(6)	11(1)
C(21)	10801(9)	13729(8)	7052(6)	10(1)
C(22)	11307(8)	12978(7)	6426(5)	7(1)
C(23)	10902(8)	11788(7)	6323(5)	6(1)
C(24)	12787(9)	14491(7)	5940(6)	9(1)
C(25)	13910(9)	14715(8)	5429(6)	9(1)
C(26)	14207(9)	15707(8)	5204(6)	10(1)
C(27)	14731(9)	14024(8)	5234(6)	10(1)
C(28)	6944(8)	9077(7)	6044(5)	7(1)
C(29)	5443(8)	8933(7)	5665(5)	5(1)
C(30)	4612(8)	9263(7)	6254(5)	7(1)
C(31)	3247(9)	9137(7)	5886(5)	7(1)
C(32)	2700(9)	8658(7)	4930(6)	9(1)
C(33)	3518(9)	8341(7)	4339(6)	9(1)
C(34)	4920(9)	8499(7)	4709(6)	8(1)
C(35)	2347(8)	9550(7)	6510(5)	7(1)

Table S3. Bond lengths [Å] and angles [°] for **2a**.

Cd-O(7)#1	2.017(6)
Cd-O(8)	2.074(6)
Cd-O(5)	2.176(6)
Cd-N(5)	2.193(7)
Cd-O(4)	2.220(6)
Cd-N(1)	2.225(7)
Cd-C(28)	2.525(8)
O(1)-C(6)	1.208(11)
O(2)-C(13)	1.230(12)
O(3)-C(24)	1.226(11)
O(4)-C(28)	1.253(10)
O(5)-C(28)	1.265(10)
O(6)-C(35)	1.253(11)
O(7)-C(35)	1.266(10)
O(8)-H(8C)	0.8500
O(8)-H(8D)	0.8500
O(9)-H(9E)	0.8501
O(9)-H(9C)	0.8497
O(10)-H(10A)	0.8500
O(10)-H(10B)	0.8499
O(12)-H(12C)	0.8500
O(12)-H(12D)	0.8504
O(13)-H(13A)	0.8499
O(13)-H(13B)	0.8498
N(1)-C(5)	1.319(11)
N(1)-C(1)	1.360(11)
N(2)-C(6)	1.377(11)
N(2)-C(4)	1.393(11)
N(2)-H(2A)	0.8600
N(3)-C(13)	1.362(12)
N(3)-C(14)	1.413(12)
N(3)-H(3A)	0.8600
N(4)-C(18)	1.339(12)
N(4)-C(17)	1.340(13)
N(5)-C(23)	1.333(10)
N(5)-C(19)	1.350(11)

Table S3. Bond lengths [Å] and angles [°] for **2a**.

N(6)-C(24)	1.362(11)
N(6)-C(22)	1.406(10)
N(6)-H(6A)	0.8600
C(1)-C(2)	1.374(13)
C(1)-H(1A)	0.9300
C(2)-C(3)	1.378(13)
C(2)-H(2B)	0.9300
C(3)-C(4)	1.398(13)
C(3)-H(3B)	0.9300
C(4)-C(5)	1.411(12)
C(5)-H(5A)	0.9300
C(6)-C(7)	1.501(12)
C(7)-C(12)	1.388(13)
C(7)-C(8)	1.408(12)
C(8)-C(9)	1.375(13)
C(8)-H(8B)	0.9300
C(9)-C(10)	1.394(13)
C(9)-H(9A)	0.9300
C(10)-C(11)	1.395(13)
C(10)-C(13)	1.491(12)
C(11)-C(12)	1.370(13)
C(11)-H(11A)	0.9300
C(12)-H(12A)	0.9300
C(14)-C(18)	1.379(13)
C(14)-C(15)	1.386(14)
C(15)-C(16)	1.398(14)
C(15)-H(15A)	0.9300
C(16)-C(17)	1.376(14)
C(16)-H(16A)	0.9300
C(17)-H(17A)	0.9300
C(18)-H(18A)	0.9300
C(19)-C(20)	1.394(12)
C(19)-H(19A)	0.9300
C(20)-C(21)	1.376(12)
C(20)-H(20A)	0.9300
C(21)-C(22)	1.404(11)

Table S3. Bond lengths [Å] and angles [°] for **2a**.

C(21)-H(21A)	0.9300
C(22)-C(23)	1.393(11)
C(23)-H(23A)	0.9300
C(24)-C(25)	1.501(11)
C(25)-C(26)	1.388(12)
C(25)-C(27)	1.392(12)
C(26)-C(27)#2	1.381(12)
C(26)-H(26A)	0.9300
C(27)-H(27A)	0.9300
C(28)-C(29)	1.511(11)
C(29)-C(34)	1.387(11)
C(29)-C(30)	1.391(11)
C(30)-C(31)	1.385(11)
C(30)-H(30A)	0.9300
C(31)-C(32)	1.386(11)
C(31)-C(35)	1.514(11)
C(32)-C(33)	1.378(12)
C(32)-H(32A)	0.9300
C(33)-C(34)	1.408(11)
C(33)-H(33A)	0.9300
C(34)-H(34A)	0.9300
O(7)#1-Cd-O(8)	99.0(2)
O(7)#1-Cd-O(5)	162.0(2)
O(8)-Cd-O(5)	98.9(2)
O(7)#1-Cd-N(5)	90.3(2)
O(8)-Cd-N(5)	87.3(2)
O(5)-Cd-N(5)	88.3(2)
O(7)#1-Cd-O(4)	102.3(2)
O(8)-Cd-O(4)	158.7(2)
O(5)-Cd-O(4)	59.8(2)
N(5)-Cd-O(4)	91.2(2)
O(7)#1-Cd-N(1)	90.5(2)
O(8)-Cd-N(1)	92.5(2)
O(5)-Cd-N(1)	90.9(2)
N(5)-Cd-N(1)	179.2(3)

Table S3. Bond lengths [Å] and angles [°] for **2a**.

O(4)-Cd-N(1)	88.6(2)
O(7)#1-Cd-C(28)	132.0(2)
O(8)-Cd-C(28)	128.9(2)
O(5)-Cd-C(28)	30.1(2)
N(5)-Cd-C(28)	88.6(3)
O(4)-Cd-C(28)	29.7(2)
N(1)-Cd-C(28)	90.8(3)
C(28)-O(4)-Cd	88.8(5)
C(28)-O(5)-Cd	90.4(5)
C(35)-O(7)-Cd#3	126.6(5)
Cd-O(8)-H(8C)	109.6
Cd-O(8)-H(8D)	109.3
H(8C)-O(8)-H(8D)	109.5
H(9E)-O(9)-H(9C)	107.9
H(10A)-O(10)-H(10B)	109.5
H(12C)-O(12)-H(12D)	109.7
H(13A)-O(13)-H(13B)	108.5
C(5)-N(1)-C(1)	117.8(7)
C(5)-N(1)-Cd	121.7(6)
C(1)-N(1)-Cd	120.2(6)
C(6)-N(2)-C(4)	125.6(7)
C(6)-N(2)-H(2A)	117.2
C(4)-N(2)-H(2A)	117.2
C(13)-N(3)-C(14)	126.6(8)
C(13)-N(3)-H(3A)	116.7
C(14)-N(3)-H(3A)	116.7
C(18)-N(4)-C(17)	118.7(9)
C(23)-N(5)-C(19)	118.3(7)
C(23)-N(5)-Cd	124.6(5)
C(19)-N(5)-Cd	117.0(5)
C(24)-N(6)-C(22)	126.6(7)
C(24)-N(6)-H(6A)	116.7
C(22)-N(6)-H(6A)	116.7
N(1)-C(1)-C(2)	122.7(8)
N(1)-C(1)-H(1A)	118.7
C(2)-C(1)-H(1A)	118.7

Table S3. Bond lengths [Å] and angles [°] for **2a**.

C(1)-C(2)-C(3)	119.2(9)
C(1)-C(2)-H(2B)	120.4
C(3)-C(2)-H(2B)	120.4
C(2)-C(3)-C(4)	119.5(9)
C(2)-C(3)-H(3B)	120.2
C(4)-C(3)-H(3B)	120.2
N(2)-C(4)-C(3)	126.3(8)
N(2)-C(4)-C(5)	116.7(8)
C(3)-C(4)-C(5)	117.0(8)
N(1)-C(5)-C(4)	123.8(8)
N(1)-C(5)-H(5A)	118.1
C(4)-C(5)-H(5A)	118.1
O(1)-C(6)-N(2)	123.1(8)
O(1)-C(6)-C(7)	121.0(8)
N(2)-C(6)-C(7)	115.9(8)
C(12)-C(7)-C(8)	119.0(8)
C(12)-C(7)-C(6)	124.0(8)
C(8)-C(7)-C(6)	116.8(8)
C(9)-C(8)-C(7)	119.8(9)
C(9)-C(8)-H(8B)	120.1
C(7)-C(8)-H(8B)	120.1
C(8)-C(9)-C(10)	120.8(8)
C(8)-C(9)-H(9A)	119.6
C(10)-C(9)-H(9A)	119.6
C(9)-C(10)-C(11)	118.9(8)
C(9)-C(10)-C(13)	123.9(8)
C(11)-C(10)-C(13)	117.2(8)
C(12)-C(11)-C(10)	120.5(9)
C(12)-C(11)-H(11A)	119.8
C(10)-C(11)-H(11A)	119.8
C(11)-C(12)-C(7)	120.9(8)
C(11)-C(12)-H(12A)	119.6
C(7)-C(12)-H(12A)	119.6
O(2)-C(13)-N(3)	122.8(8)
O(2)-C(13)-C(10)	120.3(8)
N(3)-C(13)-C(10)	116.9(8)

Table S3. Bond lengths [Å] and angles [°] for **2a**.

C(18)-C(14)-C(15)	119.8(9)
C(18)-C(14)-N(3)	115.8(9)
C(15)-C(14)-N(3)	124.3(9)
C(14)-C(15)-C(16)	117.2(9)
C(14)-C(15)-H(15A)	121.4
C(16)-C(15)-H(15A)	121.4
C(17)-C(16)-C(15)	120.0(9)
C(17)-C(16)-H(16A)	120.0
C(15)-C(16)-H(16A)	120.0
N(4)-C(17)-C(16)	121.9(9)
N(4)-C(17)-H(17A)	119.0
C(16)-C(17)-H(17A)	119.0
N(4)-C(18)-C(14)	122.3(9)
N(4)-C(18)-H(18A)	118.8
C(14)-C(18)-H(18A)	118.8
N(5)-C(19)-C(20)	121.6(8)
N(5)-C(19)-H(19A)	119.2
C(20)-C(19)-H(19A)	119.2
C(21)-C(20)-C(19)	120.3(8)
C(21)-C(20)-H(20A)	119.8
C(19)-C(20)-H(20A)	119.8
C(20)-C(21)-C(22)	118.1(8)
C(20)-C(21)-H(21A)	120.9
C(22)-C(21)-H(21A)	120.9
C(23)-C(22)-C(21)	118.2(7)
C(23)-C(22)-N(6)	117.6(7)
C(21)-C(22)-N(6)	124.1(7)
N(5)-C(23)-C(22)	123.5(7)
N(5)-C(23)-H(23A)	118.2
C(22)-C(23)-H(23A)	118.2
O(3)-C(24)-N(6)	123.5(7)
O(3)-C(24)-C(25)	120.1(7)
N(6)-C(24)-C(25)	116.4(7)
C(26)-C(25)-C(27)	118.8(8)
C(26)-C(25)-C(24)	118.2(8)
C(27)-C(25)-C(24)	122.8(8)

Table S3. Bond lengths [Å] and angles [°] for **2a**.

C(27)#2-C(26)-C(25)	120.3(8)
C(27)#2-C(26)-H(26A)	119.9
C(25)-C(26)-H(26A)	119.9
C(26)#2-C(27)-C(25)	120.9(8)
C(26)#2-C(27)-H(27A)	119.6
C(25)-C(27)-H(27A)	119.6
O(4)-C(28)-O(5)	120.9(7)
O(4)-C(28)-C(29)	119.5(7)
O(5)-C(28)-C(29)	119.6(7)
O(4)-C(28)-Cd	61.5(4)
O(5)-C(28)-Cd	59.5(4)
C(29)-C(28)-Cd	175.7(6)
C(34)-C(29)-C(30)	120.2(7)
C(34)-C(29)-C(28)	118.3(7)
C(30)-C(29)-C(28)	121.5(7)
C(31)-C(30)-C(29)	120.2(7)
C(31)-C(30)-H(30A)	119.9
C(29)-C(30)-H(30A)	119.9
C(30)-C(31)-C(32)	119.8(8)
C(30)-C(31)-C(35)	121.3(7)
C(32)-C(31)-C(35)	118.8(7)
C(33)-C(32)-C(31)	120.6(8)
C(33)-C(32)-H(32A)	119.7
C(31)-C(32)-H(32A)	119.7
C(32)-C(33)-C(34)	119.8(8)
C(32)-C(33)-H(33A)	120.1
C(34)-C(33)-H(33A)	120.1
C(29)-C(34)-C(33)	119.3(7)
C(29)-C(34)-H(34A)	120.3
C(33)-C(34)-H(34A)	120.3
O(6)-C(35)-O(7)	124.7(8)
O(6)-C(35)-C(31)	119.4(7)
O(7)-C(35)-C(31)	115.9(7)

Symmetry transformations used to generate equivalent atoms:

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