Supplementary Information

Secondary ligand-directed assembly of metal-organic coordination polymers based on 2-(pyridin-4-yl)-1H-imidazole-4,5-dicarboxylic acid ligand: syntheses, structures, photoluminescent properties

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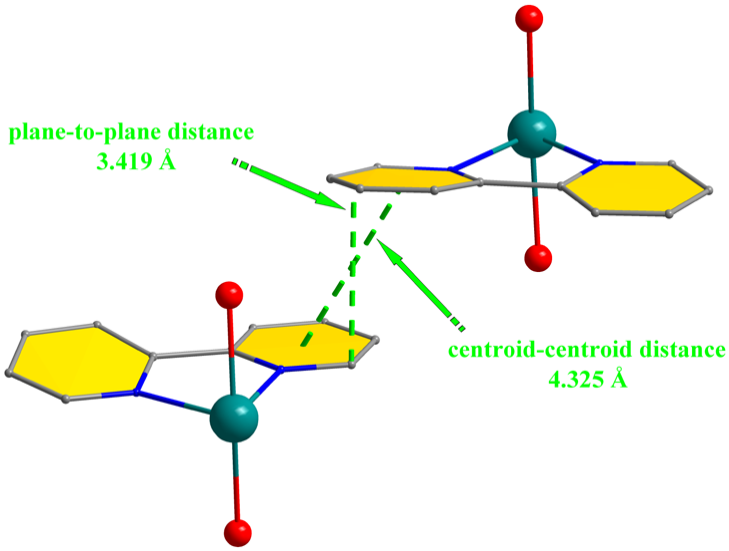

Fig. S1 The π···π interactions in complex **1.**

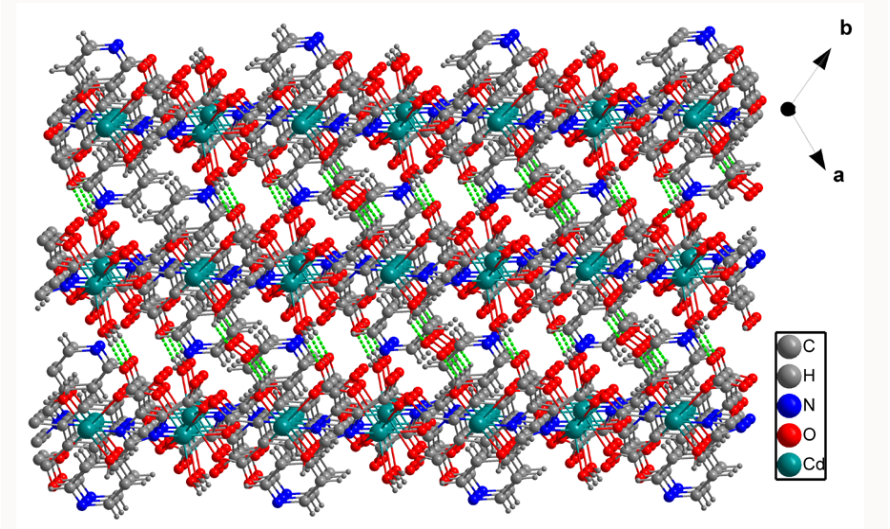

Fig. S2 The 3D supramolecular framework constructed via hydrogen bonding interactions in complex **2.**

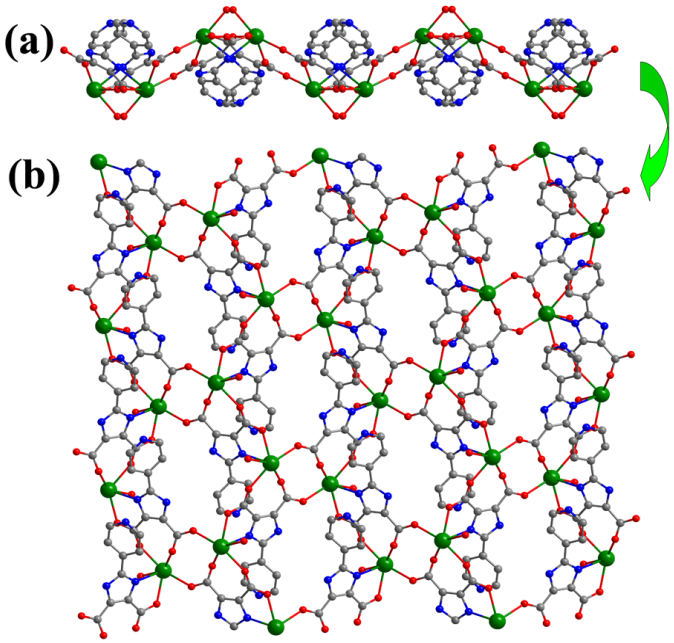

Fig. S3 The 2-D layer built by $HPIDC^{2-}$ linking Eu^{III} ions in **6** along *a*-axis (a) and *b*-axis (b).

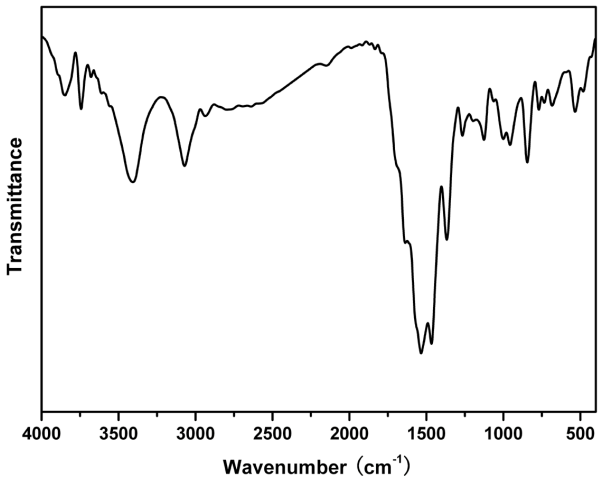

Fig. S4 Infrared spectrum of **1**.

Fig. S5 Infrared spectrum of **2**.

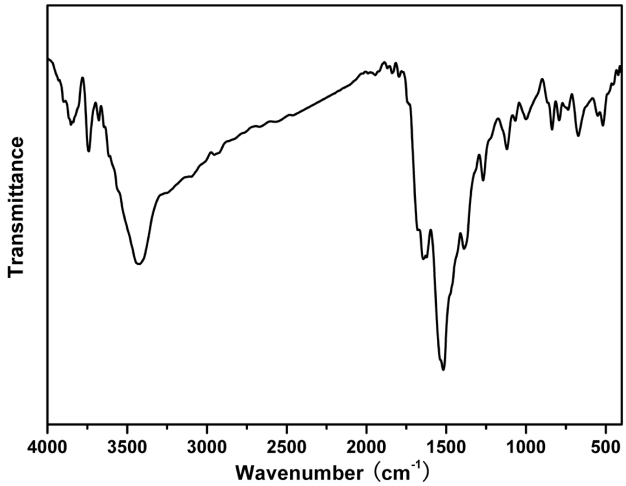

Fig. S6 Infrared spectrum of **3**.

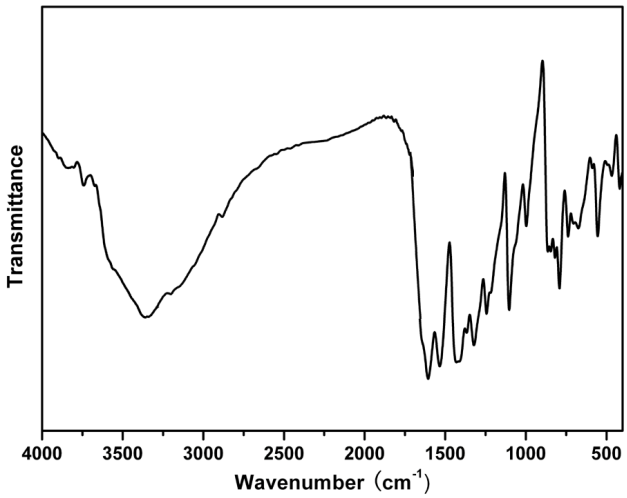

Fig. S7 Infrared spectrum of **4**.

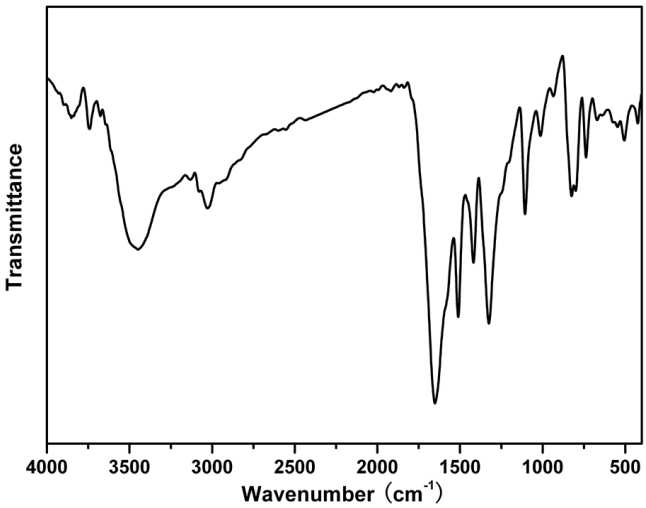

Fig. S8 Infrared spectrum of **5**.

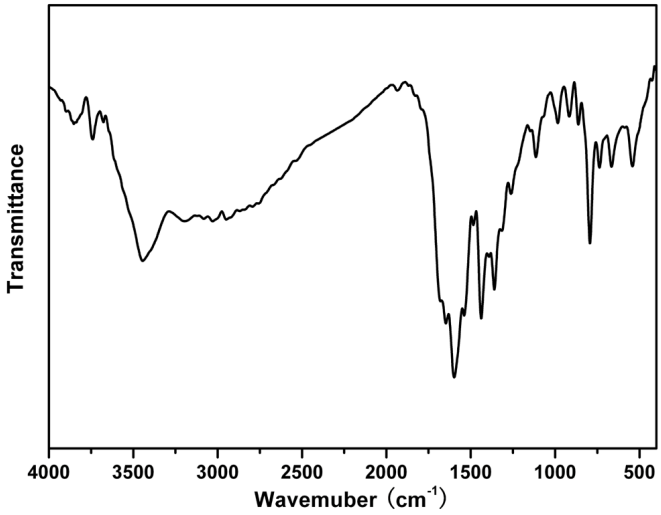

Fig. S9 Infrared spectrum of **6**.

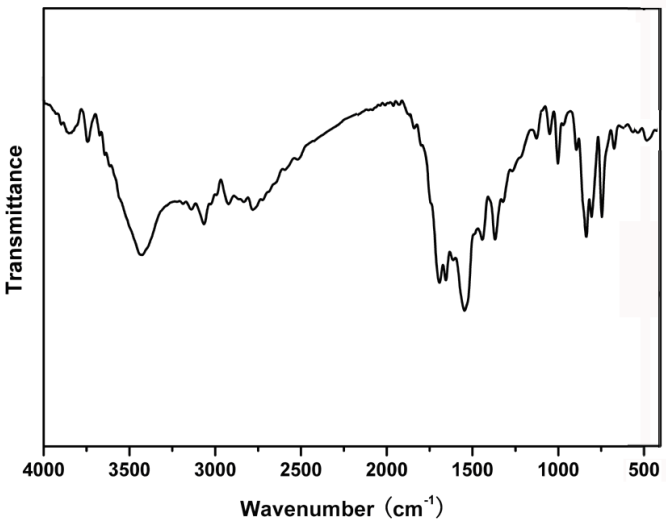

Fig. S10 Infrared spectrum of **7**.

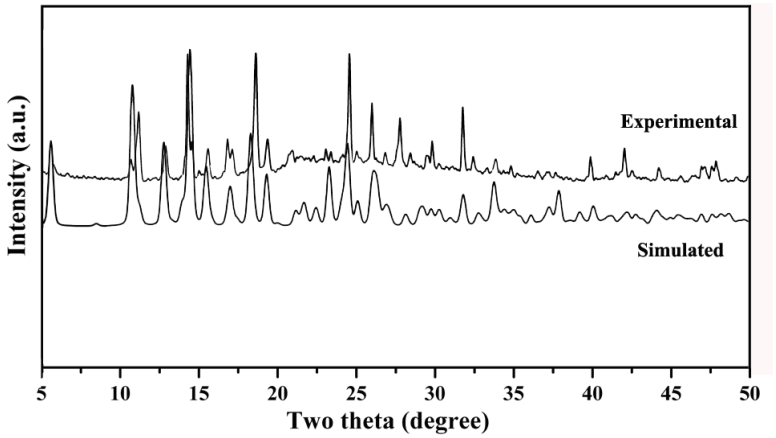

Fig. S11 Experimental and simulated XRD patterns for **1**.

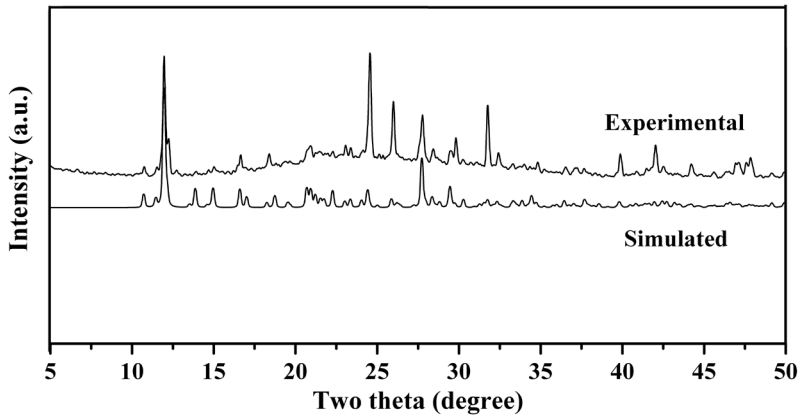

Fig. S12 Experimental and simulated XRD patterns for **2**.

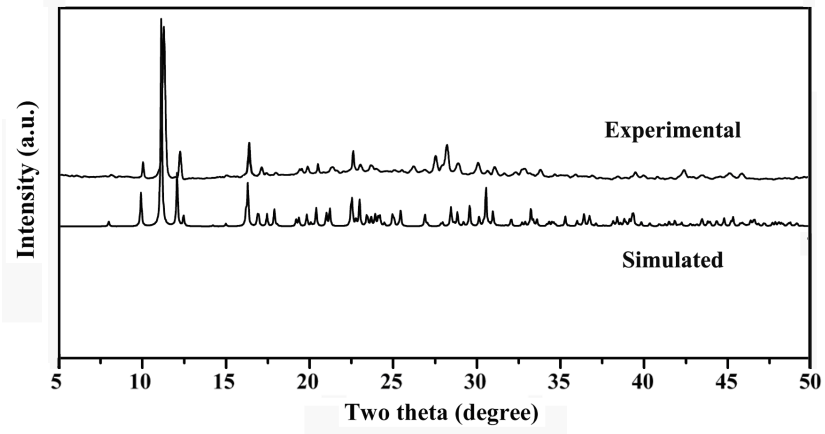

Fig. S13 Experimental and simulated XRD patterns for **3**.

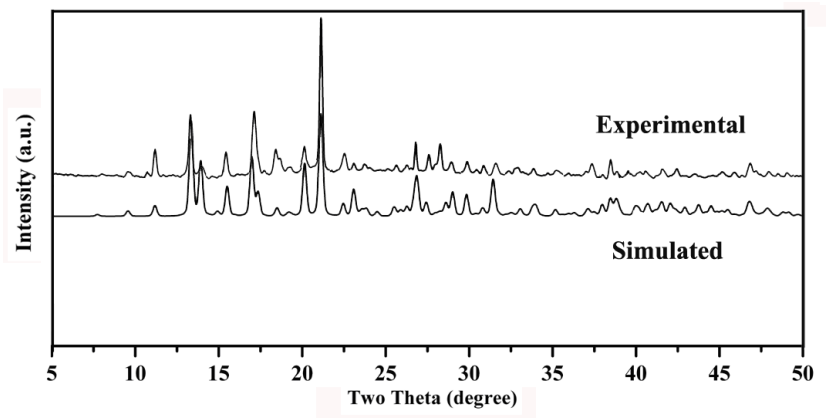

Fig. S14 Experimental and simulated XRD patterns for **4**.

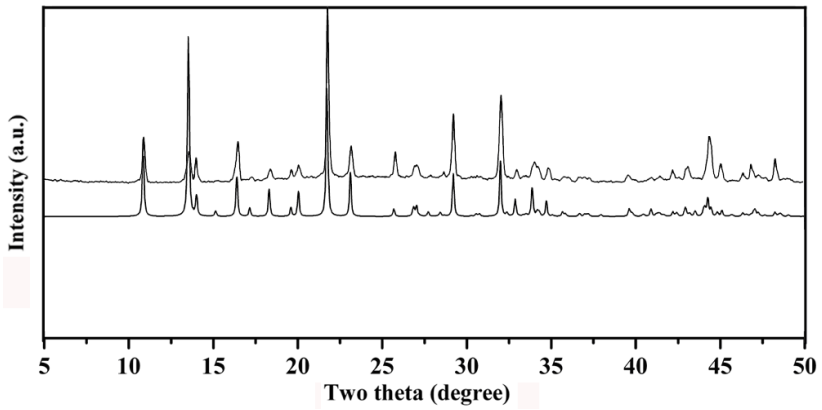

Fig. S15 Experimental and simulated XRD patterns for **5**.

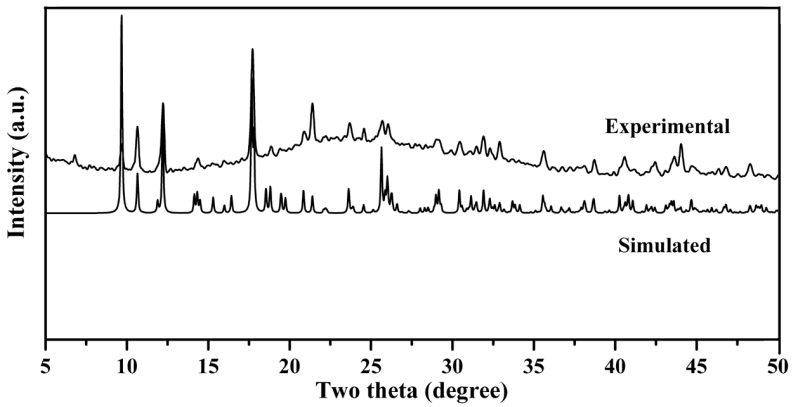

Fig. S16 Experimental and simulated XRD patterns for **6**.

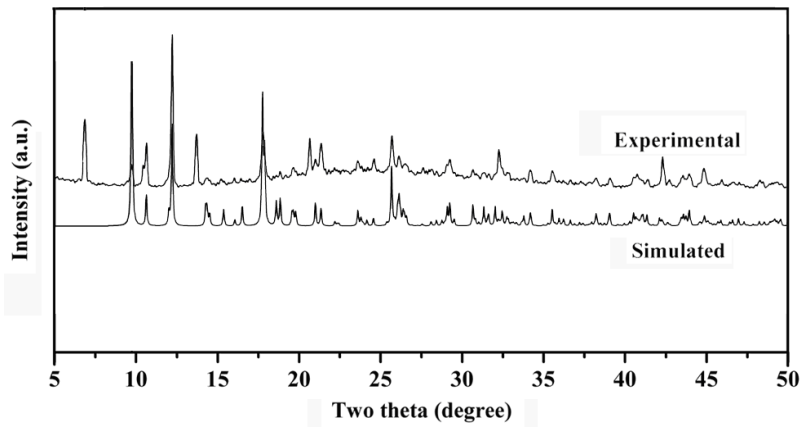

Fig. S17 Experimental and simulated XRD patterns for **7**.

Table S1. Selected bond lengths and angles for **1**–**7**.

		1	
Cd(1)-N(4)A	2.271(4)	Cd(2)-N(5)	2.285(4)
Cd(1)-N(1)	2.277(4)	Cd(2)-N(2)	2.306(4)
Cd(1)-N(3)C	2.366(4)	Cd(2)-N(7)	2.306(5)
Cd(1)-N(6)B	2.384(4)	Cd(2)-N(8)	2.319(5)
Cd(1)-O(1)	2.396(4)	Cd(2)-O(4)	2.348(4)
Cd(1)-O(5)A	2.403(4)	Cd(2)-O(8)	2.360(4)
N(4)A-Cd(1)-N(1)	143.09(13)	N(5)-Cd(2)-N(2)	83.71(14)
N(4)A-Cd(1)-N(3)C	114.36(15)	N(5)-Cd(2)-N(7)	110.15(17)
N(1)-Cd(1)-N(3)C	91.76(15)	N(2)-Cd(2)-N(7)	155.56(16)
N(4)A-Cd(1)-N(6)B	92.66(15)	N(5)-Cd(2)-N(8)	158.79(17)
N(1)-Cd(1)-N(6)B	113.18(16)	N(2)-Cd(2)-N(8)	102.31(17)
N(3)C-Cd(1)-N(6)B	91.55(14)	N(7)-Cd(2)-N(8)	72.24(19)
N(4)A-Cd(1)-O(1)	84.25(14)	N(5)-Cd(2)-O(4)	114.74(15)
N(1)-Cd(1)-O(1)	72.27(15)	N(2)-Cd(2)-O(4)	73.24(14)
N(3)C-Cd(1)-O(1)	84.51(15)	N(7)-Cd(2)-O(4)	82.57(15)
N(6)B-Cd(1)-O(1)	173.44(15)	N(8)-Cd(2)-O(4)	86.43(17)
N(4)A-Cd(1)-O(5)A	72.25(15)	N(5)-Cd(2)-O(8)	73.15(14)
N(1)-Cd(1)-O(5)A	83.12(15)	N(2)-Cd(2)-O(8)	116.57(15)
N(3)C-Cd(1)-O(5)A	173.18(15)	N(7)-Cd(2)-O(8)	87.23(16)
N(6)B-Cd(1)-O(5)A	86.37(16)	N(8)-Cd(2)-O(8)	86.09(16)
O(1)-Cd(1)-O(5)A	98.14(12)	O(4)-Cd(2)-O(8)	168.81(12)
		2	
Cd(1)-O(4)	2.293(3)	Cd(2)-O(1W)	2.327(4)
Cd(1)-O(2W)	2.328(4)	Cd(2)-N(1)	2.338(4)
Cd(1)-N(2)	2.337(3)	Cd(2)-O(1)	2.350(3)
Cd(2)-O(8)	2.238(3)	Cd(2)-O(5)B	2.407(3)
Cd(2)-O(7)C	2.243(3)		
O(4)A-Cd(1)-O(4)	180.000(1)	O(8)-Cd(2)-N(1)	146.15(12)

O(4)-Cd(1)-O(2W)A	91.00(15)	O(7)C-Cd(2)-N(1)	110.79(12)
O(4)-Cd(1)-O(2W)	89.00(15)	O(1W)-Cd(2)-N(1)	87.35(13)
O(2W)A-Cd(1)-O(2W)	180.000(1)	O(8)-Cd(2)-O(1)	78.90(12)
O(4)A-Cd(1)-N(2)	106.15(11)	O(7)C-Cd(2)-O(1)	162.62(12)
O(4)-Cd(1)-N(2)	73.85(11)	O(1W)-Cd(2)-O(1)	110.08(12)
O(2W)A-Cd(1)-N(2)	87.10(15)	N(1)-Cd(2)-O(1)	72.20(11)
O(2W)-Cd(1)-N(2)	92.90(15)	O(8)-Cd(2)-O(5)B	113.38(12)
N(2)-Cd(1)-N(2)A	180.000(1)	O(7)C-Cd(2)-O(5)B	78.98(11)
O(8)-Cd(2)-O(7)C	102.08(12)	O(1W)-Cd(2)-O(5)B	157.82(11)
O(8)-Cd(2)-O(1W)	86.33(13)	N(1)-Cd(2)-O(5)B	81.48(12)
O(7)C-Cd(2)-O(1W)	87.27(12)	O(1)-Cd(2)-O(5)B	84.70(11)

3

Cd(1)-N(3)C	2.281(4)	Cd(2)-O(1W)	2.225(4)
Cd(1)-N(1)	2.313(3)	Cd(2)-N(2)	2.283(3)
Cd(1)-O(1)	2.313(3)	Cd(2)-O(5)	2.290(3)
Cd(1)-O(6)A	2.360(3)	Cd(2)-O(4)	2.386(3)
Cd(1)-Cl(1)	2.6059(18)	Cd(2)-O(5)D	2.520(3)
Cd(1)-Cl(1)B	2.6939(15)	Cd(2)-Cl(1)E	2.7430(16)
N(3)C-Cd(1)-N(1)	99.75(12)	O(1W)-Cd(2)-N(2)	93.17(13)
N(3)C-Cd(1)-O(1)	170.26(12)	O(1W)-Cd(2)-O(5)	106.45(14)
N(1)-Cd(1)-O(1)	73.81(11)	N(2)-Cd(2)-O(5)	155.83(12)
N(3)C-Cd(1)-O(6)A	96.91(13)	O(1W)-Cd(2)-O(4)	160.51(12)
N(1)-Cd(1)-O(6)A	100.29(11)	N(2)-Cd(2)-O(4)	72.08(11)
O(1)-Cd(1)-O(6)A	91.51(12)	O(5)-Cd(2)-O(4)	85.43(11)
N(3)C-Cd(1)-Cl(1)	94.69(9)	O(1W)-Cd(2)-O(5)D	89.34(14)
N(1)-Cd(1)-Cl(1)	165.54(8)	N(2)-Cd(2)-O(5)D	95.35(11)
O(1)-Cd(1)-Cl(1)	91.97(8)	O(5)-Cd(2)-O(5)D	71.42(11)
O(6)A-Cd(1)-Cl(1)	76.98(8)	O(4)-Cd(2)-O(5)D	79.73(11)
N(3)C-Cd(1)-Cl(1)B	87.19(10)	O(1W)-Cd(2)-Cl(1)E	100.66(12)
N(1)-Cd(1)-Cl(1)B	96.51(9)	N(2)-Cd(2)-Cl(1)E	82.46(9)
O(1)-Cd(1)-Cl(1)B	86.32(10)	O(5)-Cd(2)-Cl(1)E	106.92(8)
O(6)A-Cd(1)-Cl(1)B	161.74(8)	O(4)-Cd(2)-Cl(1)E	90.18(9)
Cl(1)-Cd(1)-Cl(1)B	84.98(3)	O(5)D-Cd(2)-Cl(1)E	169.85(8)

4

Cd(1)-O(6)B	2.249(3)	Cd(2)-N(1)	2.238(4)
Cd(1)-O(3)C	2.253(3)	Cd(2)-O(1W)	2.265(4)
Cd(1)-N(2)D	2.294(4)	Cd(2)-O(2)A	2.297(3)
Cd(1)-N(3)	2.307(4)	Cd(2)-O(1)	2.446(3)
Cd(1)-O(4)D	2.318(3)	Cd(2)-O(1)A	2.533(4)
Cd(2)-O(5)	2.213(4)		
O(6)B-Cd(1)-O(3)C	85.85(12)	O(5)-Cd(2)-O(2)A	89.99(13)
O(6)B-Cd(1)-N(2)D	115.00(12)	N(1)-Cd(2)-O(2)A	144.87(13)
O(3)C-Cd(1)-N(2)D	156.39(13)	O(1W)-Cd(2)-O(2)A	93.98(14)
O(6)B-Cd(1)-N(3)	91.77(14)	O(5)-Cd(2)-O(1)	171.98(13)

O(3)C-Cd(1)-N(3)	96.27(13)	N(1)-Cd(2)-O(1)	70.14(12)
N(2)D-Cd(1)-N(3)	94.09(13)	O(1W)-Cd(2)-O(1)	78.69(15)
O(6)B-Cd(1)-O(4)D	100.95(12)	O(2)A-Cd(2)-O(1)	94.50(12)
O(3)C-Cd(1)-O(4)D	92.99(12)	O(5)-Cd(2)-O(1)A	90.60(13)
N(2)D-Cd(1)-O(4)D	73.03(11)	N(1)-Cd(2)-O(1)A	95.60(12)
N(3)-Cd(1)-O(4)D	164.78(13)	O(1W)-Cd(2)-O(1)A	147.63(14)
O(5)-Cd(2)-N(1)	109.46(13)	O(2)A-Cd(2)-O(1)A	54.00(10)
O(5)-Cd(2)-O(1W)	94.39(16)	O(1)-Cd(2)-O(1)A	97.41(6)
N(1)-Cd(2)-O(1W)	112.61(15)		

5

Zn(1)-O(3)	2.013(4)	Zn(1)-N(1)	2.078(4)
Zn(1)-O(1W)	2.055(4)	Zn(1)-O(4)A	2.171(4)
Zn(1)-O(1)	2.066(4)	Zn(1)-O(1)C	2.216(4)
O(3)-Zn(1)-O(1W)	101.07(17)	O(1)-Zn(1)-O(4)A	84.27(16)
O(3)-Zn(1)-O(1)	163.54(16)	N(1)-Zn(1)-O(4)A	90.34(17)
O(1W)-Zn(1)-O(1)	92.75(18)	O(3)-Zn(1)-O(1)C	89.66(15)
O(3)-Zn(1)-N(1)	106.87(16)	O(1W)-Zn(1)-O(1)C	89.61(17)
O(1W)-Zn(1)-N(1)	98.58(18)	O(1)-Zn(1)-O(1)C	81.46(16)
O(1)-Zn(1)-N(1)	79.52(15)	N(1)-Zn(1)-O(1)C	159.60(16)
O(3)-Zn(1)-O(4)A	80.59(15)	O(4)A-Zn(1)-O(1)C	80.46(16)
O(1W)-Zn(1)-O(4)A	169.95(17)		

6

Eu(1)-O(2)B	2.308(4)	Eu(1)-O(1W)	2.415(4)
Eu(1)-O(3)B	2.362(3)	Eu(1)-O(5)	2.433(4)
Eu(1)-O(1)	2.391(3)	Eu(1)-O(6)C	2.443(3)
Eu(1)-O(4)A	2.401(3)	Eu(1)-N(2)A	2.567(4)
O(2)B-Eu(1)-O(3)B	75.29(12)	O(1W)-Eu(1)-O(5)	73.22(15)
O(2)B-Eu(1)-O(1)	76.77(12)	O(2)B-Eu(1)-O(6)C	78.47(13)
O(3)B-Eu(1)-O(1)	152.00(13)	O(3)B-Eu(1)-O(6)C	76.27(12)
O(2)B-Eu(1)-O(4)A	128.67(13)	O(1)-Eu(1)-O(6)C	99.91(14)
O(3)B-Eu(1)-O(4)A	126.66(11)	O(4)A-Eu(1)-O(6)C	145.39(12)
O(1)-Eu(1)-O(4)A	71.46(12)	O(1W)-Eu(1)-O(6)C	93.68(14)
O(2B-Eu(1)-O(1W)	147.47(12)	O(5)-Eu(1)-O(6)C	66.54(12)
O(3)B-Eu(1)-O(1W)	72.18(12)	O(2)B-Eu(1)-N(2)A	84.49(13)
O(1)-Eu(1)-O(1W)	135.74(12)	O(3)B-Eu(1)-N(2)A	74.20(12)
O(4)A-Eu(1)-O(1W)	73.58(12)	O(1)-Eu(1)-N(2)A	101.38(15)
O(2)B-Eu(1)-O(5)	128.92(13)	O(4)A-Eu(1)-N(2)A	64.20(12)
O(3)B-Eu(1)-O(5)	126.43(13)	O(1W)-Eu(1)-N(2)A	86.78(14)
O(1)-Eu(1)-O(5)	74.15(15)	O(5)-Eu(1)-N(2)A	141.86(12)
O(4)A-Eu(1)-O(5)	78.92(12)	O(6)C-Eu(1)-N(2)A	148.79(12)

7

Tb(1)-O(3)A	2.274(5)	Tb(1)-O(1)	2.373(4)
Tb(1)-O(2)A	2.341(4)	Tb(1)-O(5)	2.400(4)
Tb(1)-O(4)A	2.364(4)	Tb(1)-O(6)C	2.418(4)

Tb(1)-O(1W)	2.365(5)	Tb(1)-N(2)	2.536(5)
O(3)A-Tb(1)-O(2)A	76.14(15)	O(1)-Tb(1)-O(5)	78.07(15)
O(3)A-Tb(1)-O(4)B	76.06(16)	O(3)A-Tb(1)-O(6)C	78.91(17)
O(2)A-Tb(1)-O(4)B	152.15(16)	O(2)A-Tb(1)-O(6)C	76.29(15)
O(3)A-Tb(1)-O(1W)	147.78(17)	O(4)B-Tb(1)-O(6)C	99.70(17)
O(2)A-Tb(1)-O(1W)	71.65(16)	O(1W)-Tb(1)-O(6)C	92.65(19)
O(4)B-Tb(1)-O(1W)	136.17(17)	O(1)-Tb(1)-O(6)C	144.88(15)
O(3)A-Tb(1)-O(1)	128.77(16)	O(5)-Tb(1)-O(6)C	66.95(14)
O(2)A-Tb(1)-O(1)	126.38(15)	O(3)A-Tb(1)-N(2)	84.31(17)
O(4)B-Tb(1)-O(1)	72.08(15)	O(2)A-Tb(1)-N(2)	74.09(16)
O(1W)-Tb(1)-O(1)	73.81(17)	O(4)B-Tb(1)-N(2)	101.68(18)
O(3)A-Tb(1)-O(5)	128.73(17)	O(1W)-Tb(1)-N(2)	87.59(19)
O(2)A-Tb(1)-O(5)	126.88(16)	O(1)-Tb(1)-N(2)	64.67(15)
O(4)B-Tb(1)-O(5)	73.53(18)	O(5)-Tb(1)-N(2)	141.68(16)
O(1W)-Tb(1)-O(5)	73.16(19)	O(6)C-Tb(1)-N(2)	148.67(15)

Symmetry code: For **1,** A: -x, -y+1, z+1/2; B: x+1/2,-y+1,z; C:-x+1/2, y, z+1/2. For **2**, A: -x, -y, -z+2; B: x-1, y-1, z; C: -x+1, -y+1, -z+1; D: -x+2, -y+2, -z+1. For **3,** A: x, y+1, z; B: -x+1, -y+3, -z; C: -x+2, -y+2, -z; D: -x+1, -y+1, -z+1; E: x, y-1, z; F: -x+1, -y, -z +1. For **4,** A: -x+3/2, y +1/2, -z+1/2; B: x, y+1, z; C: x-1/2, -y+3/2, z-1/2; D: -x+2, -y+2, -z. For **5,** A: -x+1/2, -y+1/2, -z; B: -x+1, y, -z+1/2; C: -x+1, -y+1, -z. For **6,** A: -x+2, y+1/2, -z+31/2; B: -x+2, -y+2, -z+2; C: -x+1, -y+2, -z+2. For **7,** A: x, -y+1/2, z+1/2; B: -x+2, y-1/2, -z+3/2; C: -x+1, -y, -z+2.