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Supporting Information for

Weak interactions cause selective cocrystal form of lanthanide nitrates and tetra-2-pyridinylpyrazine

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Table S1. Hydrogen-bonding geometry for **1-Eu** and **2-Er**.

	D-H···A (Å)	H···A (Å)	D−H (Å)	angle of DHA (deg.)
1-Eu	C_1-H_{1a}···O8	2.3899(23)	0.9929(36)	136.313(227)
	C_2-H_{2a}···O_9	2.5565(7)	0.9293(34)	159.025(218)
	C_3-H_{3a}···O_5	2.6700(33)	0.9297(39)	119.984(234)
	C_4-H_{4b}···O_5	2.5322(32)	0.9308(35)	125.898(238)
	C_{10}-H_{10a}···O_1	2.5646(36)	0.9298(37)	151.482(244)
	C_{11}-H_{11a}···O_3	2.4457(35)	0.9296(37)	165.259(239)
	C_{12}-H_{12a}···O_6	2.5340(34)	0.9303(34)	145.597(231)
2-Er	C_1-H_{1a}···O_8	2.9857(30)	0.9290(57)	156.348(320)
	C_2-H_{2a}···O_{14}	2.4420(23)	0.9302(50)	161.213(319)
	C_9-H_{9b}···O_2	2.5177(23)	0.9296(36)	122.920(219)
	C_{10}-H_{10b}···O_{13}	2.9293(37)	0.9303(34)	132.597(244)
	C_{11}-H_{11a}···O_5	2.7312(34)	0.9296(36)	95.232(270)
	C_{13}-H_{13a}···O_9	2.6259(34)	0.9299(35)	104.819(219)
	C_{16}-H_{16a}···O_3	2.8002(26)	0.9309(35)	134.586(236)
	C_{22}-H_{22a}···O_1	2.7181(29)	0.9303(34)	145.448(258)
	C_{24}-H_{24a}···O_{10}	2.3754(28)	0.9298(46)	163.742(245)

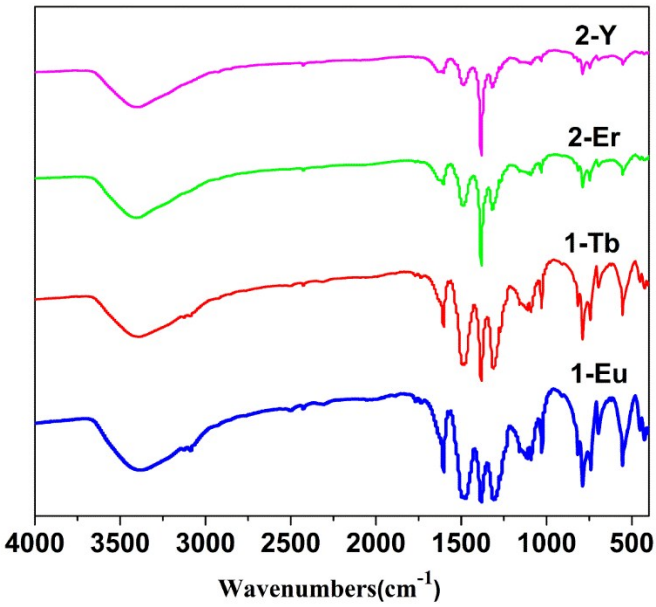

Fig. S1. FT-IR spectra of the two series of lanthanide cocrystals.

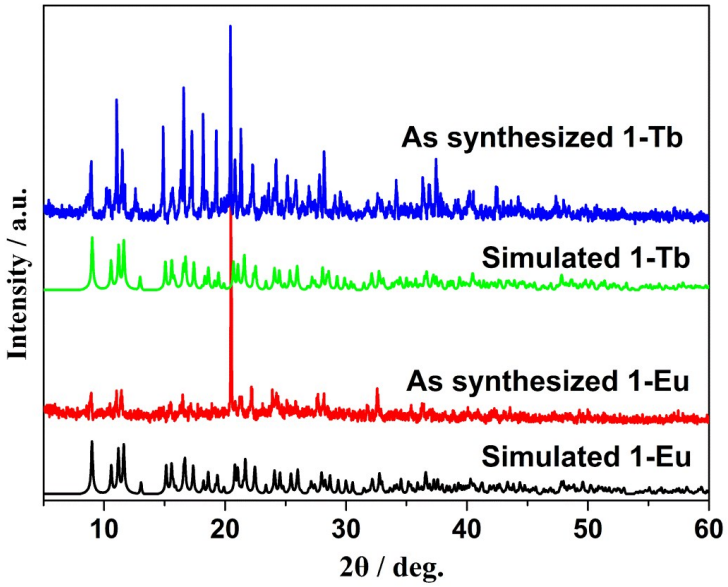

Fig. S2. PXRD comparisons of bulk samples of **1-Eu**, **1-Tb** and their corresponding simulated results from single-crystal data.

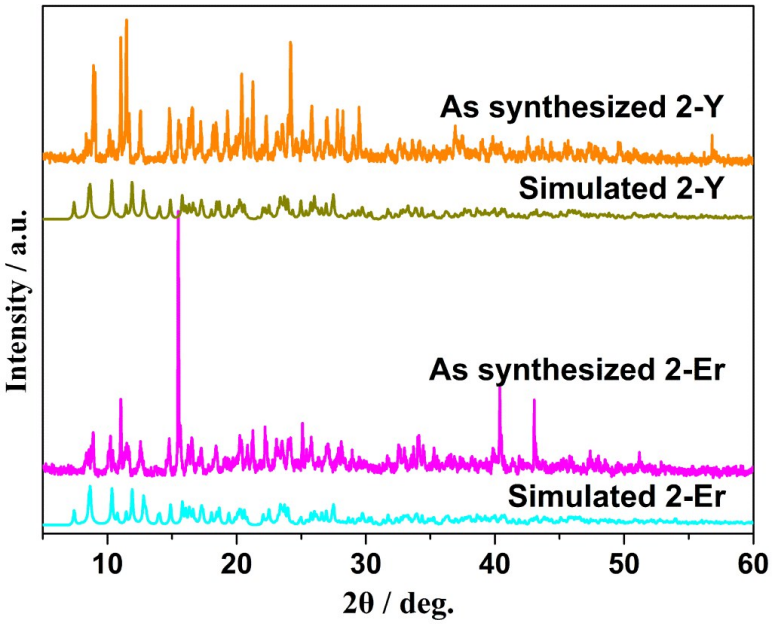

Fig. S3. PXRD comparisons of bulk samples of **2-Er**, **2-Y** and their corresponding simulated results from single-crystal data.

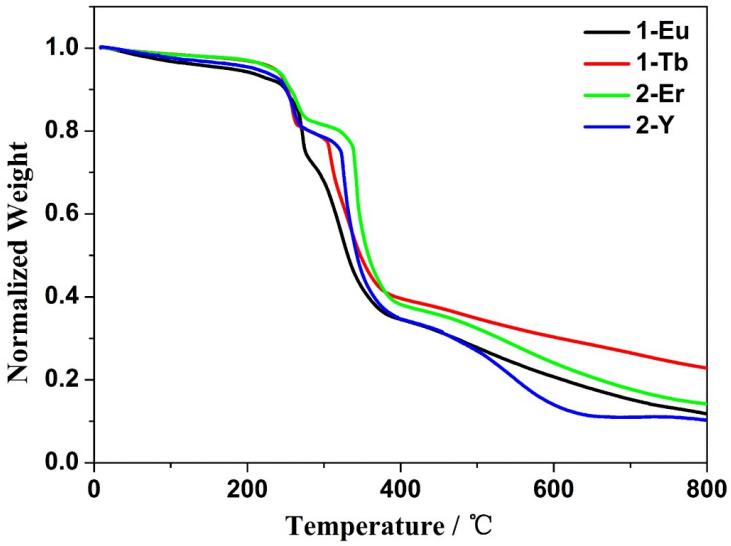

Fig. S4. TGA of the two series of lanthanide cocrystals in the atmosphere, from room temperature to 800 °C.

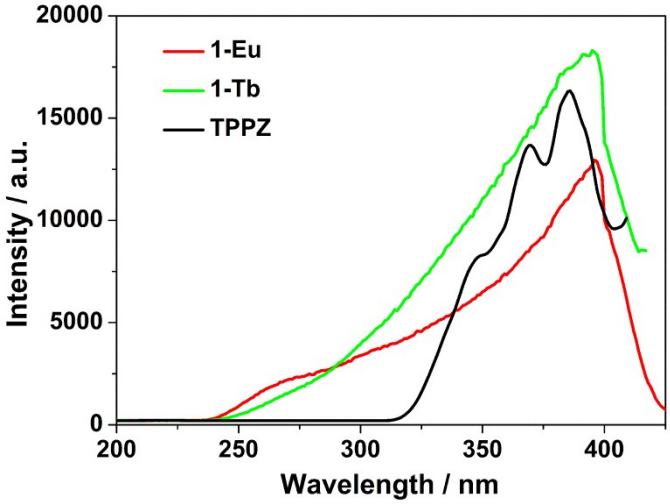

Fig. S5. The excitation spectra of the ligand TPPZ, **1-Eu** and **1-Tb** in solid state.

Table S2. Bond lengths [Å] and bond angles [deg] for **1-Eu**.

N(4)-C(1)	1.336(5)	Eu(1)-O(5)#2	2.454(3)
N(4)-C(5)	1.337(4)	Eu(1)-O(5)	2.454(3)
N(4)-H(4A)	0.8600	Eu(1)-O(2)#2	2.471(4)
N(5)-C(12)	1.338(5)	Eu(1)-O(2)	2.471(4)
N(5)-C(8)	1.345(4)	Eu(1)-O(4)	2.477(4)
N(6)-C(7)#1	1.331(4)	Eu(1)-O(4)#2	2.477(4)
N(6)-C(6)	1.332(4)	Eu(1)-O(8)	2.502(3)
C(7)-N(6)#1	1.331(4)	Eu(1)-O(8)#2	2.502(3)
C(7)-C(6)	1.426(5)	Eu(1)-O(1)	2.529(4)
C(7)-C(8)	1.497(5)	Eu(1)-O(1)#2	2.529(4)
C(8)-C(9)	1.386(5)	Eu(1)-N(2)#2	2.894(3)
C(6)-C(5)	1.502(4)	Eu(1)-N(2)	2.894(3)
C(5)-C(4)	1.393(5)	O(8)-N(3)	1.271(3)
C(4)-C(3)	1.384(5)	N(1)-O(1)	1.252(5)
C(4)-H(4B)	0.9300	N(1)-O(2)	1.242(5)
C(3)-C(2)	1.382(6)	N(1)-O(3)	1.223(5)
C(3)-H(3A)	0.9300	O(9)-N(3)	1.233(5)
C(10)-C(9)	1.394(5)	N(3)-O(8)#2	1.271(3)
C(10)-C(11)	1.386(6)	O(6)-N(2)	1.217(4)
C(10)-H(10A)	0.9300	N(2)-O(5)	1.255(5)
C(12)-C(11)	1.374(6)	N(2)-O(4)	1.276(4)
C(12)-H(12A)	0.9300	C(2)-C(1)	1.380(6)
C(11)-H(11A)	0.9300	C(2)-H(2A)	0.9300
C(9)-H(9A)	0.9300	C(1)-H(1A)	0.9300
C(1)-N(4)-C(5)	121.6(3)	O(2)-Eu(1)-O(8)#2	73.24(13)
C(1)-N(4)-H(4A)	119.2	O(4)-Eu(1)-O(8)#2	118.94(9)
C(5)-N(4)-H(4A)	119.2	O(4)#2-Eu(1)-O(8)#2	67.76(9)
C(12)-N(5)-C(8)	121.8(3)	O(8)-Eu(1)-O(8)#2	51.24(12)
C(7)#1-N(6)-C(6)	123.6(3)	O(5)#2-Eu(1)-O(1)	68.81(12)
N(6)#1-C(7)-C(6)	117.9(3)	O(5)-Eu(1)-O(1)	73.90(13)
N(6)#1-C(7)-C(8)	111.3(3)	O(2)#2-Eu(1)-O(1)	159.30(16)
C(6)-C(7)-C(8)	130.8(3)	O(2)-Eu(1)-O(1)	49.77(11)
N(5)-C(8)-C(9)	119.0(3)	O(4)-Eu(1)-O(1)	106.24(16)

N(5)-C(8)-C(7)	119.9(3)	O(4)#2-Eu(1)-O(1)	70.96(16)
C(9)-C(8)-C(7)	121.1(3)	O(8)-Eu(1)-O(1)	118.21(10)
N(6)-C(6)-C(7)	118.4(3)	O(8)#2-Eu(1)-O(1)	104.20(12)
N(6)-C(6)-C(5)	110.9(3)	O(5)#2-Eu(1)-O(1)#2	73.90(13)
C(7)-C(6)-C(5)	130.7(3)	O(5)-Eu(1)-O(1)#2	68.81(12)
N(4)-C(5)-C(4)	119.5(3)	O(2)#2-Eu(1)-O(1)#2	49.77(11)
N(4)-C(5)-C(6)	119.9(3)	O(2)-Eu(1)-O(1)#2	159.30(16)
C(4)-C(5)-C(6)	120.6(3)	O(4)-Eu(1)-O(1)#2	70.96(15)
C(5)-C(4)-C(3)	119.4(3)	O(4)#2-Eu(1)-O(1)#2	106.24(16)
C(5)-C(4)-H(4B)	120.3	O(8)-Eu(1)-O(1)#2	104.20(12)
C(3)-C(4)-H(4B)	120.3	O(8)#2-Eu(1)-O(1)#2	118.21(10)
C(2)-C(3)-C(4)	119.8(4)	O(1)-Eu(1)-O(1)#2	133.08(19)
C(2)-C(3)-H(3A)	120.1	O(5)#2-Eu(1)-N(2)#2	25.49(10)
C(4)-C(3)-H(3A)	120.1	O(5)-Eu(1)-N(2)#2	97.17(11)
C(9)-C(10)-C(11)	119.4(4)	O(2)#2-Eu(1)-N(2)#2	93.98(15)
C(9)-C(10)-H(10A)	120.3	O(2)-Eu(1)-N(2)#2	106.46(12)
C(11)-C(10)-H(10A)	120.3	O(4)-Eu(1)-N(2)#2	147.35(10)
N(5)-C(12)-C(11)	121.5(3)	O(4)#2-Eu(1)-N(2)#2	26.02(10)
N(5)-C(12)-H(12A)	119.2	O(8)-Eu(1)-N(2)#2	144.60(9)
C(11)-C(12)-H(12A)	119.2	O(8)#2-Eu(1)-N(2)#2	93.40(9)
C(12)-C(11)-C(10)	118.4(3)	O(1)-Eu(1)-N(2)#2	66.59(11)
C(12)-C(11)-H(11A)	120.8	O(1)#2-Eu(1)-N(2)#2	90.64(13)
C(10)-C(11)-H(11A)	120.8	O(5)#2-Eu(1)-N(2)	97.17(11)
C(10)-C(9)-C(8)	119.9(3)	O(5)-Eu(1)-N(2)	25.49(10)
C(10)-C(9)-H(9A)	120.1	O(2)#2-Eu(1)-N(2)	106.46(12)
C(8)-C(9)-H(9A)	120.1	O(2)-Eu(1)-N(2)	93.98(15)
C(3)-C(2)-C(1)	118.3(3)	O(4)-Eu(1)-N(2)	26.02(10)
C(3)-C(2)-H(2A)	120.8	O(4)#2-Eu(1)-N(2)	147.35(10)
C(1)-C(2)-H(2A)	120.8	O(8)-Eu(1)-N(2)	93.40(9)
N(4)-C(1)-C(2)	121.3(4)	O(8)#2-Eu(1)-N(2)	144.60(9)
N(4)-C(1)-H(1A)	119.3	O(1)-Eu(1)-N(2)	90.64(13)
C(2)-C(1)-H(1A)	119.3	O(1)#2-Eu(1)-N(2)	66.59(11)
O(5)#2-Eu(1)-O(5)	73.32(16)	N(2)#2-Eu(1)-N(2)	121.99(14)
O(5)#2-Eu(1)-O(2)#2	96.95(15)	N(3)-O(8)-Eu(1)	96.0(2)

O(5)-Eu(1)-O(2)#2	117.55(11)	O(1)-N(1)-O(2)	115.1(4)
O(5)#2-Eu(1)-O(2)	117.55(11)	O(1)-N(1)-O(3)	121.9(4)
O(5)-Eu(1)-O(2)	96.95(15)	O(2)-N(1)-O(3)	122.9(4)
O(2)#2-Eu(1)-O(2)	137.34(18)	O(1)-N(1)-Eu(1)	59.3(2)
O(5)#2-Eu(1)-O(4)	121.95(10)	O(2)-N(1)-Eu(1)	56.5(2)
O(5)-Eu(1)-O(4)	51.48(10)	O(3)-N(1)-Eu(1)	174.9(3)
O(2)#2-Eu(1)-O(4)	93.98(17)	O(9)-N(3)-O(8)#2	121.64(19)
O(2)-Eu(1)-O(4)	88.46(17)	O(9)-N(3)-O(8)	121.64(19)
O(5)#2-Eu(1)-O(4)#2	51.48(10)	O(8)#2-N(3)-O(8)	116.7(4)
O(5)-Eu(1)-O(4)#2	121.95(10)	O(9)-N(3)-Eu(1)	180.0
O(2)#2-Eu(1)-O(4)#2	88.46(17)	O(8)#2-N(3)-Eu(1)	58.36(19)
O(2)-Eu(1)-O(4)#2	93.98(17)	O(8)-N(3)-Eu(1)	58.36(19)
O(4)-Eu(1)-O(4)#2	173.30(14)	O(6)-N(2)-O(5)	122.6(4)
O(5)#2-Eu(1)-O(8)	167.32(11)	O(6)-N(2)-O(4)	121.8(4)
O(5)-Eu(1)-O(8)	118.10(10)	O(5)-N(2)-O(4)	115.6(3)
O(2)#2-Eu(1)-O(8)	73.24(13)	O(6)-N(2)-Eu(1)	174.8(3)
O(2)-Eu(1)-O(8)	68.44(10)	O(5)-N(2)-Eu(1)	57.27(19)
O(4)-Eu(1)-O(8)	67.76(9)	O(4)-N(2)-Eu(1)	58.4(2)
O(4)#2-Eu(1)-O(8)	118.94(9)	N(2)-O(4)-Eu(1)	95.6(3)
O(5)#2-Eu(1)-O(8)#2	118.10(10)	N(1)-O(1)-Eu(1)	95.5(2)
O(5)-Eu(1)-O(8)#2	167.32(11)	N(1)-O(2)-Eu(1)	98.7(3)
O(2)#2-Eu(1)-O(8)#2	68.44(10)	N(2)-O(5)-Eu(1)	97.2(2)

Symmetrytransformationsusedtogenerateequivalentatoms: #1 -x+1/2, -y+1/2, -z; #2 -x, y, -z+1/2.

Table S3. Bond lengths [Å] and bond angles [deg] for **1-Tb**.

N(5)-C(8)	1.336(6)	Tb(1)-O(5)#2	2.426(4)
N(5)-C(12)	1.344(6)	Tb(1)-O(5)	2.426(4)
N(4)-C(5)	1.342(6)	Tb(1)-O(4)	2.446(5)
N(4)-C(1)	1. 338(6)	Tb(1)-O(4)#2	2.446(5)
C(6)-N(6)#1	1.335(6)	Tb(1)-O(1)#2	2.455(5)
C(6)-C(7)	1.423(6)	Tb(1)-O(1)	2.455(5)
C(6)-C(5)	1.496(6)	Tb(1)-O(7)#2	2.481(4)
N(6)-C(7)	1.328(6)	Tb(1)-O(7)	2.481(3)
N(6)-C(6)#1	1.335(6)	Tb(1)-O(2)#2	2.496(5)
C(7)-C(8)	1.509(6)	Tb(1)-O(2)	2.496(5)
C(5)-C(4)	1.388(7)	Tb(1)-N(2)#2	2.872(4)
C(12)-C(11)	1.373(8)	Tb(1)-N(2)	2.872(4)
C(12)-H(12)	0.9300	O(7)-N(3)	1.264(4)
C(4)-C(3)	1.388(7)	O(8)-N(3)	1.232(7)
C(4)-H(4)	0.9300	O(3)-N(1)	1.212(7)
C(8)-C(9)	1.391(7)	N(1)-O(1)	1.218(7)
C(10)-C(9)	1.397(7)	N(1)-O(2)	1.256(7)
C(10)-C(11)	1.388(7)	N(3)-O(7)#2	1.264(4)
C(10)-H(10)	0.9300	O(6)-N(2)	1.209(6)
C(3)-C(2)	1.378(8)	O(4)-N(2)	1.279(6)
C(3)-H(3)	0.9300	N(2)-O(5)	1.244(6)
C(11)-H(11)	0.9300	C(1)-H(1)	0.9300
C(9)-H(9)	0.9300	C(2)-H(2)	0.9300
C(1)-C(2)	1.388(8)		
C(8)-N(5)-C(12)	121.3(4)	O(1)#2-Tb(1)-O(7)	73.27(19)
C(5)-N(4)-C(1)	121.1(5)	O(1)-Tb(1)-O(7)	68.72(14)
N(6)#1-C(6)-C(7)	118.2(4)	O(7)#2-Tb(1)-O(7)	51.45(16)
N(6)#1-C(6)-C(5)	110.9(4)	O(5)#2-Tb(1)-O(2)#2	68.74(18)
C(7)-C(6)-C(5)	130.9(4)	O(5)-Tb(1)-O(2)#2	74.0(2)
C(7)-N(6)-C(6)#1	123.5(4)	O(4)-Tb(1)-O(2)#2	105.3(3)
N(6)-C(7)-C(6)	118.3(4)	O(4)#2-Tb(1)-O(2)#2	71.9(3)
N(6)-C(7)-C(8)	111.2(4)	O(1)#2-Tb(1)-O(2)#2	49.50(17)
C(6)-C(7)-C(8)	130.5(4)	O(1)-Tb(1)-O(2)#2	159.3(3)

N(4)-C(5)-C(4)	119.7(4)	O(7)#2-Tb(1)-O(2)#2	118.22(15)
N(4)-C(5)-C(6)	119.6(4)	O(7)-Tb(1)-O(2)#2	103.89(19)
C(4)-C(5)-C(6)	120.8(4)	O(5)#2-Tb(1)-O(2)	73.9(2)
N(5)-C(12)-C(11)	122.2(5)	O(5)-Tb(1)-O(2)	68.74(18)
N(5)-C(12)-H(12)	118.9	O(4)-Tb(1)-O(2)	71.9(3)
C(11)-C(12)-H(12)	118.9	O(4)#2-Tb(1)-O(2)	105.3(3)
C(5)-C(4)-C(3)	120.0(5)	O(1)#2-Tb(1)-O(2)	159.3(3)
C(5)-C(4)-H(4)	120.0	O(1)-Tb(1)-O(2)	49.50(17)
C(3)-C(4)-H(4)	120.0	O(7)#2-Tb(1)-O(2)	103.89(19)
N(5)-C(8)-C(9)	119.6(4)	O(7)-Tb(1)-O(2)	118.22(15)
N(5)-C(8)-C(7)	120.1(4)	O(2)#2-Tb(1)-O(2)	133.4(3)
C(9)-C(8)-C(7)	120.3(4)	O(5)#2-Tb(1)-N(2)#2	25.43(13)
C(9)-C(10)-C(11)	119.7(5)	O(5)-Tb(1)-N(2)#2	96.46(14)
C(9)-C(10)-H(10)	120.1	O(4)-Tb(1)-N(2)#2	147.02(14)
C(11)-C(10)-H(10)	120.1	O(4)#2-Tb(1)-N(2)#2	26.30(14)
C(2)-C(3)-C(4)	119.1(5)	O(1)#2-Tb(1)-N(2)#2	107.39(17)
C(2)-C(3)-H(3)	120.4	O(1)-Tb(1)-N(2)#2	93.1(2)
C(4)-C(3)-H(3)	120.4	O(7)#2-Tb(1)-N(2)#2	144.97(12)
C(12)-C(11)-C(10)	117.8(4)	O(7)-Tb(1)-N(2)#2	93.62(12)
C(12)-C(11)-H(11)	121.1	O(2)#2-Tb(1)-N(2)#2	67.49(17)
C(10)-C(11)-H(11)	121.1	O(2)-Tb(1)-N(2)#2	89.7(2)
C(10)-C(9)-C(8)	119.4(4)	O(5)#2-Tb(1)-N(2)	96.46(14)
C(10)-C(9)-H(9)	120.3	O(5)-Tb(1)-N(2)	25.43(13)
C(8)-C(9)-H(9)	120.3	O(4)-Tb(1)-N(2)	26.30(14)
N(4)-C(1)-C(2)	121.4(5)	O(4)#2-Tb(1)-N(2)	147.02(14)
N(4)-C(1)-H(1)	119.3	O(1)#2-Tb(1)-N(2)	93.1(2)
C(2)-C(1)-H(1)	119.3	O(1)-Tb(1)-N(2)	107.39(17)
C(3)-C(2)-C(1)	118.7(5)	O(7)#2-Tb(1)-N(2)	93.62(12)
C(3)-C(2)-H(2)	120.6	O(7)-Tb(1)-N(2)	144.97(12)
C(1)-C(2)-H(2)	120.6	O(2)#2-Tb(1)-N(2)	89.7(2)
O(5)#2-Tb(1)-O(5)	72.3(2)	O(2)-Tb(1)-N(2)	67.49(17)
O(5)#2-Tb(1)-O(4)	121.63(15)	N(2)#2-Tb(1)-N(2)	121.39(18)
O(5)-Tb(1)-O(4)	51.72(15)	N(3)-O(7)-Tb(1)	95.8(3)
O(5)#2-Tb(1)-O(4)#2	51.72(15)	O(3)-N(1)-O(1)	124.2(5)

O(5)-Tb(1)-O(4)#2	121.63(15)	O(3)-N(1)-O(2)	121.7(5)
O(4)-Tb(1)-O(4)#2	173.2(2)	O(1)-N(1)-O(2)	113.9(5)
O(5)#2-Tb(1)-O(1)#2	117.34(17)	O(3)-N(1)-Tb(1)	175.4(5)
O(5)-Tb(1)-O(1)#2	97.1(2)	O(1)-N(1)-Tb(1)	56.3(3)
O(4)-Tb(1)-O(1)#2	87.5(3)	O(2)-N(1)-Tb(1)	58.5(3)
O(4)#2-Tb(1)-O(1)#2	95.0(3)	O(8)-N(3)-O(7)#2	121.5(3)
O(5)#2-Tb(1)-O(1)	97.1(2)	O(8)-N(3)-O(7)	121.5(3)
O(5)-Tb(1)-O(1)	117.34(17)	O(7)#2-N(3)-O(7)	116.9(5)
O(4)-Tb(1)-O(1)	95.0(3)	O(8)-N(3)-Tb(1)	180.0
O(4)#2-Tb(1)-O(1)	87.5(3)	O(7)#2-N(3)-Tb(1)	58.5(3)
O(1)#2-Tb(1)-O(1)	137.7(3)	O(7)-N(3)-Tb(1)	58.5(3)
O(5)#2-Tb(1)-O(7)#2	167.83(15)	N(2)-O(4)-Tb(1)	95.8(3)
O(5)-Tb(1)-O(7)#2	118.52(13)	O(6)-N(2)-O(5)	123.1(5)
O(4)-Tb(1)-O(7)#2	67.66(13)	O(6)-N(2)-O(4)	122.1(5)
O(4)#2-Tb(1)-O(7)#2	119.10(13)	O(5)-N(2)-O(4)	114.7(5)
O(1)#2-Tb(1)-O(7)#2	68.72(14)	O(6)-N(2)-Tb(1)	175.3(4)
O(1)-Tb(1)-O(7)#2	73.27(19)	O(5)-N(2)-Tb(1)	56.8(2)
O(5)#2-Tb(1)-O(7)	118.52(13)	O(4)-N(2)-Tb(1)	57.9(3)
O(5)-Tb(1)-O(7)	167.83(15)	N(1)-O(2)-Tb(1)	96.2(4)
O(4)-Tb(1)-O(7)	119.10(13)	N(2)-O(5)-Tb(1)	97.7(3)
O(4)#2-Tb(1)-O(7)	67.66(13)	N(1)-O(1)-Tb(1)	99.4(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, -y+1/2, -z; #2 -x, y, -z+1/2.

Table S4. Bond lengths [Å] and bond angles [deg] for **2-Er**.

C(15)-C(16)	1.383(5)	Er(1)-O(1)	2.401(2)
C(15)-C(14)	1.382(6)	Er(1)-O(5)	2.413(3)
C(15)-H(15A)	0.9300	Er(1)-O(4)	2.415(2)
N(10)-C(17)	1.345(4)	Er(1)-O(14)	2.417(2)
N(10)-C(13)	1.351(4)	Er(1)-O(8)	2.417(3)
N(9)-C(18)	1.327(4)	Er(1)-O(10)	2.429(3)
N(9)-C(19)	1.331(4)	Er(1)-O(7)	2.438(3)
C(18)-C(19)#1	1.426(5)	Er(1)-O(11)	2.440(3)
C(18)-C(17)	1.494(4)	Er(1)-O(2)	2.448(3)
C(17)-C(16)	1.395(5)	Er(1)-O(13)	2.462(2)
C(16)-H(16A)	0.9300	Er(1)-N(2)	2.844(3)
C(13)-C(14)	1.374(5)	Er(1)-N(1)	2.849(3)
C(13)-H(13A)	0.9300	N(4)-O(12)	1.221(4)
C(14)-H(14A)	0.9300	N(4)-O(10)	1.267(4)
C(1)-N(7)	1.344(5)	N(4)-O(11)	1.271(4)
C(1)-C(2)	1.368(7)	N(2)-O(6)	1.211(4)
C(1)-H(1A)	0.9300	N(2)-O(5)	1.269(4)
C(2)-C(3)	1.373(7)	N(2)-O(4)	1.275(4)
C(2)-H(2A)	0.9300	O(2)-N(1)	1.268(4)
C(10)-C(11)	1.378(6)	O(7)-N(3)	1.271(4)
C(10)-C(9)	1.384(5)	O(8)-N(3)	1.272(4)
C(10)-H(10B)	0.9300	O(13)-N(5)	1.270(4)
C(12)-N(8)	1.345(5)	O(9)-N(3)	1.226(4)
C(12)-C(11)	1.356(6)	O(15)-N(5)	1.216(4)
C(12)-H(12A)	0.9300	N(5)-O(14)	1.282(4)
N(7)-C(5)	1.342(5)	O(1)-N(1)	1.279(4)
C(5)-C(4)	1.386(5)	N(1)-O(3)	1.218(4)
C(5)-C(6)	1.504(5)	N(6)-C(7)#2	1.330(4)
C(4)-C(3)	1.390(6)	C(19)-C(18)#1	1.426(5)
C(4)-H(4A)	0.9300	C(19)-C(20)	1.494(5)
C(3)-H(3A)	0.9300	C(20)-N(11)	1.341(4)
C(6)-N(6)	1.334(4)	C(20)-C(21)	1.394(5)
C(6)-C(7)	1.416(5)	C(21)-C(22)	1.379(5)

C(7)-N(6)#2	1.330(4)	C(21)-H(21A)	0.9300
C(7)-C(8)	1.490(5)	N(11)-C(24)	1.340(5)
C(9)-C(8)	1.381(5)	C(24)-C(23)	1.374(5)
C(9)-H(9B)	0.9300	C(24)-H(24A)	0.9300
C(11)-H(11A)	0.9300	C(22)-C(23)	1.388(5)
N(8)-C(8)	1.352(4)	C(22)-H(22A)	0.9300
C(23)-H(23A)	0.9300		
C(16)-C(15)-C(14)	120.0(3)	O(7)-Er(1)-O(2)	172.55(8)
C(16)-C(15)-H(15A)	120.0	O(11)-Er(1)-O(2)	107.68(9)
C(14)-C(15)-H(15A)	120.0	O(1)-Er(1)-O(13)	123.53(9)
C(17)-N(10)-C(13)	121.0(3)	O(5)-Er(1)-O(13)	71.58(9)
C(18)-N(9)-C(19)	123.2(3)	O(4)-Er(1)-O(13)	118.64(8)
N(9)-C(18)-C(19)#1	118.6(3)	O(14)-Er(1)-O(13)	52.49(8)
N(9)-C(18)-C(17)	111.5(3)	O(8)-Er(1)-O(13)	163.11(9)
C(19)#1-C(18)-C(17)	129.9(3)	O(10)-Er(1)-O(13)	94.12(9)
N(10)-C(17)-C(16)	119.8(3)	O(7)-Er(1)-O(13)	116.29(9)
N(10)-C(17)-C(18)	120.3(3)	O(11)-Er(1)-O(13)	72.26(9)
C(16)-C(17)-C(18)	119.9(3)	O(2)-Er(1)-O(13)	70.94(9)
C(15)-C(16)-C(17)	119.2(3)	O(1)-Er(1)-N(2)	79.74(9)
C(15)-C(16)-H(16A)	120.4	O(5)-Er(1)-N(2)	26.34(8)
C(17)-C(16)-H(16A)	120.4	O(4)-Er(1)-N(2)	26.47(8)
N(10)-C(13)-C(14)	121.2(3)	O(14)-Er(1)-N(2)	77.49(8)
N(10)-C(13)-H(13A)	119.4	O(8)-Er(1)-N(2)	97.68(9)
C(14)-C(13)-H(13A)	119.4	O(10)-Er(1)-N(2)	151.93(8)
C(13)-C(14)-C(15)	118.8(3)	O(7)-Er(1)-N(2)	93.55(9)
C(13)-C(14)-H(14A)	120.6	O(11)-Er(1)-N(2)	155.51(8)
C(15)-C(14)-H(14A)	120.6	O(2)-Er(1)-N(2)	87.34(9)
N(7)-C(1)-C(2)	121.8(4)	O(13)-Er(1)-N(2)	95.67(8)
N(7)-C(1)-H(1A)	119.1	O(1)-Er(1)-N(1)	26.48(9)
C(2)-C(1)-H(1A)	119.1	O(5)-Er(1)-N(1)	77.50(9)
C(1)-C(2)-C(3)	118.9(4)	O(4)-Er(1)-N(1)	94.24(9)
C(1)-C(2)-H(2A)	120.5	O(14)-Er(1)-N(1)	141.89(9)
C(3)-C(2)-H(2A)	120.5	O(8)-Er(1)-N(1)	94.33(10)
C(11)-C(10)-C(9)	120.2(4)	O(10)-Er(1)-N(1)	68.34(9)

C(11)-C(10)-H(10B)	119.9	O(7)-Er(1)-N(1)	146.42(9)
C(9)-C(10)-H(10B)	119.9	O(11)-Er(1)-N(1)	117.69(9)
N(8)-C(12)-C(11)	121.0(4)	O(2)-Er(1)-N(1)	26.32(9)
N(8)-C(12)-H(12A)	119.5	O(13)-Er(1)-N(1)	97.25(9)
C(11)-C(12)-H(12A)	119.5	N(2)-Er(1)-N(1)	84.34(9)
C(5)-N(7)-C(1)	119.9(4)	O(12)-N(4)-O(10)	122.3(3)
N(7)-C(5)-C(4)	121.1(3)	O(12)-N(4)-O(11)	122.3(3)
N(7)-C(5)-C(6)	118.9(3)	O(10)-N(4)-O(11)	115.4(3)
C(4)-C(5)-C(6)	119.9(3)	O(12)-N(4)-Er(1)	179.0(3)
C(5)-C(4)-C(3)	118.3(4)	O(10)-N(4)-Er(1)	57.42(16)
C(5)-C(4)-H(4A)	120.8	O(11)-N(4)-Er(1)	57.93(16)
C(3)-C(4)-H(4A)	120.8	O(6)-N(2)-O(5)	122.3(3)
C(2)-C(3)-C(4)	120.0(4)	O(6)-N(2)-O(4)	122.7(3)
C(2)-C(3)-H(3A)	120.0	O(5)-N(2)-O(4)	115.0(3)
C(4)-C(3)-H(3A)	120.0	O(6)-N(2)-Er(1)	176.5(2)
N(6)-C(6)-C(7)	117.8(3)	O(5)-N(2)-Er(1)	57.49(16)
N(6)-C(6)-C(5)	111.8(3)	O(4)-N(2)-Er(1)	57.62(15)
C(7)-C(6)-C(5)	130.4(3)	N(1)-O(2)-Er(1)	94.8(2)
N(6)#2-C(7)-C(6)	119.0(3)	N(3)-O(7)-Er(1)	95.2(2)
N(6)#2-C(7)-C(8)	111.0(3)	N(3)-O(8)-Er(1)	96.16(19)
C(6)-C(7)-C(8)	130.0(3)	N(5)-O(13)-Er(1)	94.83(18)
C(8)-C(9)-C(10)	119.0(4)	N(2)-O(5)-Er(1)	96.17(19)
C(8)-C(9)-H(9B)	120.5	N(4)-O(10)-Er(1)	96.50(19)
C(10)-C(9)-H(9B)	120.5	N(2)-O(4)-Er(1)	95.90(18)
C(12)-C(11)-C(10)	119.1(4)	O(9)-N(3)-O(7)	122.2(3)
C(12)-C(11)-H(11A)	120.5	O(9)-N(3)-O(8)	122.1(3)
C(10)-C(11)-H(11A)	120.5	O(7)-N(3)-O(8)	115.7(3)
C(12)-N(8)-C(8)	121.3(3)	O(9)-N(3)-Er(1)	174.3(2)
N(8)-C(8)-C(9)	119.6(3)	O(7)-N(3)-Er(1)	58.43(16)
N(8)-C(8)-C(7)	119.7(3)	O(8)-N(3)-Er(1)	57.50(16)
C(9)-C(8)-C(7)	120.8(3)	O(15)-N(5)-O(13)	122.6(3)
O(1)-Er(1)-O(5)	84.98(10)	O(15)-N(5)-O(14)	122.0(3)
O(1)-Er(1)-O(4)	78.65(9)	O(13)-N(5)-O(14)	115.5(3)
O(5)-Er(1)-O(4)	52.76(9)	O(15)-N(5)-Er(1)	173.7(2)

O(1)-Er(1)-O(14)	156.09(9)	O(13)-N(5)-Er(1)	58.94(15)
O(5)-Er(1)-O(14)	71.35(9)	O(14)-N(5)-Er(1)	56.94(15)
O(4)-Er(1)-O(14)	84.16(8)	N(5)-O(14)-Er(1)	96.67(18)
O(1)-Er(1)-O(8)	69.34(9)	N(4)-O(11)-Er(1)	95.87(19)
O(5)-Er(1)-O(8)	123.21(9)	N(1)-O(1)-Er(1)	96.70(19)
O(4)-Er(1)-O(8)	72.49(9)	O(3)-N(1)-O(2)	122.7(3)
O(14)-Er(1)-O(8)	120.92(9)	O(3)-N(1)-O(1)	121.8(3)
O(1)-Er(1)-O(10)	72.92(9)	O(2)-N(1)-O(1)	115.4(3)
O(5)-Er(1)-O(10)	141.00(9)	O(3)-N(1)-Er(1)	175.2(3)
O(4)-Er(1)-O(10)	145.12(9)	O(2)-N(1)-Er(1)	58.89(16)
O(14)-Er(1)-O(10)	128.41(8)	O(1)-N(1)-Er(1)	56.82(15)
O(8)-Er(1)-O(10)	78.77(9)	C(7)#2-N(6)-C(6)	123.2(3)
O(1)-Er(1)-O(7)	120.17(9)	N(9)-C(19)-C(18)#1	118.2(3)
O(5)-Er(1)-O(7)	113.40(9)	N(9)-C(19)-C(20)	111.6(3)
O(4)-Er(1)-O(7)	71.98(9)	C(18)#1-C(19)-C(20)	130.1(3)
O(14)-Er(1)-O(7)	68.77(9)	N(11)-C(20)-C(21)	119.7(3)
O(8)-Er(1)-O(7)	52.63(9)	N(11)-C(20)-C(19)	119.7(3)
O(10)-Er(1)-O(7)	105.50(9)	C(21)-C(20)-C(19)	120.5(3)
O(1)-Er(1)-O(11)	124.73(9)	C(22)-C(21)-C(20)	119.5(3)
O(5)-Er(1)-O(11)	142.25(9)	C(22)-C(21)-H(21A)	120.2
O(4)-Er(1)-O(11)	145.57(9)	C(20)-C(21)-H(21A)	120.2
O(14)-Er(1)-O(11)	78.32(8)	C(24)-N(11)-C(20)	121.1(3)
O(8)-Er(1)-O(11)	91.47(9)	N(11)-C(24)-C(23)	121.7(3)
O(10)-Er(1)-O(11)	52.28(8)	N(11)-C(24)-H(24A)	119.2
O(7)-Er(1)-O(11)	74.10(9)	C(23)-C(24)-H(24A)	119.2
O(1)-Er(1)-O(2)	52.71(9)	C(21)-C(22)-C(23)	119.7(3)
O(5)-Er(1)-O(2)	69.86(9)	C(21)-C(22)-H(22A)	120.1
O(4)-Er(1)-O(2)	106.72(9)	C(23)-C(22)-H(22A)	120.1
O(14)-Er(1)-O(2)	118.60(9)	C(24)-C(23)-C(22)	118.3(3)
O(8)-Er(1)-O(2)	119.92(9)	C(24)-C(23)-H(23A)	120.8
O(10)-Er(1)-O(2)	71.17(9)	C(22)-C(23)-H(23A)	120.8

Symmetrytransformationsusedtogenerateequivalentatoms: #1 -x+2, -y+3, -z+1; #2 -x+1, -y+2, -z.

Table S5. Bond lengths [Å] and bond angles [deg] for **2-Y**.

N(9)-C(17)	1.341(4)	C(1)-H(1)	0.9300
N(9)-C(13)	1.347(4)	C(7)-C(8)	1.501(5)
N(6)-C(1)	1.346(5)	C(4)-C(3)	1.394(5)
N(6)-C(5)	1.355(4)	C(4)-H(4)	0.9300
N(7)-C(8)	1.342(5)	C(9)-C(10)	1.383(6)
N(7)-C(12)	1.347(5)	C(9)-C(8)	1.386(5)
Y(2)-O(1)	2.421(3)	C(9)-H(9)	0.9300
Y(2)-O(14)	2.425(3)	C(3)-C(2)	1.373(6)
Y(2)-O(8)	2.434(2)	C(3)-H(3)	0.9300
Y(2)-O(11)	2.435(3)	C(2)-H(2)	0.9300
Y(2)-O(13)	2.437(3)	C(12)-C(11)	1.377(7)
Y(2)-O(4)	2.443(3)	C(12)-H(12)	0.9300
Y(2)-O(10)	2.450(3)	C(10)-C(11)	1.379(7)
Y(2)-O(2)	2.461(3)	C(10)-H(10)	0.9300
Y(2)-O(5)	2.464(3)	C(11)-H(11)	0.9300
Y(2)-O(7)	2.475(3)	C(17)-C(16)	1.393(5)
Y(2)-N(5)	2.860(3)	C(17)-C(18)	1.492(4)
Y(2)-N(1)	2.870(3)	C(18)-N(11)	1.340(4)
N(5)-O(15)	1.219(4)	C(18)-C(19)	1.417(4)
N(5)-O(13)	1.261(4)	C(13)-C(14)	1.371(5)
N(5)-O(14)	1.282(4)	C(13)-H(13)	0.9300
N(2)-O(6)	1.219(4)	C(15)-C(16)	1.382(5)
N(2)-O(5)	1.261(4)	C(15)-C(14)	1.386(5)
N(2)-O(4)	1.286(4)	C(15)-H(15)	0.9300
O(10)-N(4)	1.273(4)	C(14)-H(14)	0.9300
O(2)-N(1)	1.275(4)	C(16)-H(16)	0.9300
O(8)-N(3)	1.278(4)	N(10)-C(24)	1.342(5)
O(7)-N(3)	1.274(4)	N(10)-C(20)	1.342(4)
O(11)-N(4)	1.277(4)	C(20)-C(21)	1.402(5)
N(3)-O(9)	1.219(4)	C(20)-C(19)	1.494(5)
O(12)-N(4)	1.216(4)	C(21)-C(22)	1.375(5)
O(1)-N(1)	1.276(4)	C(21)-H(21)	0.9300
N(1)-O(3)	1.210(4)	C(22)-C(23)	1.389(5)

N(8)-C(7)	1.331(4)	C(22)-H(22)	0.9300
N(8)-C(6)#1	1.337(4)	C(23)-C(24)	1.378(5)
C(6)-N(8)#1	1.337(4)	C(23)-H(23)	0.9300
C(6)-C(7)	1.422(5)	C(24)-H(24)	0.9300
C(6)-C(5)	1.486(5)	N(11)-C(19)#2	1.334(4)
C(5)-C(4)	1.379(5)	C(19)-N(11)#2	1.334(4)
C(1)-C(2)	1.370(6)		
C(17)-N(9)-C(13)	121.5(3)	O(7)-N(3)-O(8)	115.8(3)
C(1)-N(6)-C(5)	121.5(3)	O(9)-N(3)-Y(2)	174.1(3)
C(8)-N(7)-C(12)	120.1(4)	O(7)-N(3)-Y(2)	58.99(16)
O(1)-Y(2)-O(14)	78.69(9)	O(8)-N(3)-Y(2)	57.20(15)
O(1)-Y(2)-O(8)	156.89(9)	N(1)-O(1)-Y(2)	96.9(2)
O(14)-Y(2)-O(8)	84.76(9)	O(12)-N(4)-O(10)	122.4(3)
O(1)-Y(2)-O(11)	69.20(10)	O(12)-N(4)-O(11)	122.2(3)
O(14)-Y(2)-O(11)	72.36(9)	O(10)-N(4)-O(11)	115.4(3)
O(8)-Y(2)-O(11)	120.81(9)	O(12)-N(4)-Y(2)	174.4(2)
O(1)-Y(2)-O(13)	85.99(10)	O(10)-N(4)-Y(2)	58.15(16)
O(14)-Y(2)-O(13)	52.44(8)	O(11)-N(4)-Y(2)	57.47(16)
O(8)-Y(2)-O(13)	71.10(9)	O(3)-N(1)-O(2)	122.5(3)
O(11)-Y(2)-O(13)	123.07(9)	O(3)-N(1)-O(1)	122.2(3)
O(1)-Y(2)-O(4)	72.41(9)	O(2)-N(1)-O(1)	115.3(3)
O(14)-Y(2)-O(4)	144.86(9)	O(3)-N(1)-Y(2)	174.8(3)
O(8)-Y(2)-O(4)	128.13(8)	O(2)-N(1)-Y(2)	58.66(16)
O(11)-Y(2)-O(4)	78.91(9)	O(1)-N(1)-Y(2)	56.89(16)
O(13)-Y(2)-O(4)	141.54(9)	C(7)-N(8)-C(6)#1	123.1(3)
O(1)-Y(2)-O(10)	119.94(9)	N(8)#1-C(6)-C(7)	118.7(3)
O(14)-Y(2)-O(10)	72.28(9)	N(8)#1-C(6)-C(5)	110.9(3)
O(8)-Y(2)-O(10)	68.88(9)	C(7)-C(6)-C(5)	130.4(3)
O(11)-Y(2)-O(10)	52.38(9)	N(6)-C(5)-C(4)	119.6(3)
O(13)-Y(2)-O(10)	112.92(9)	N(6)-C(5)-C(6)	119.3(3)
O(4)-Y(2)-O(10)	105.44(9)	C(4)-C(5)-C(6)	121.0(3)
O(1)-Y(2)-O(2)	52.39(9)	N(6)-C(1)-C(2)	120.6(4)
O(14)-Y(2)-O(2)	105.80(9)	N(6)-C(1)-H(1)	119.7
O(8)-Y(2)-O(2)	118.80(9)	C(2)-C(1)-H(1)	119.7

O(11)-Y(2)-O(2)	119.78(9)	N(8)-C(7)-C(6)	118.2(3)
O(13)-Y(2)-O(2)	70.06(10)	N(8)-C(7)-C(8)	111.6(3)
O(4)-Y(2)-O(2)	71.55(9)	C(6)-C(7)-C(8)	130.2(3)
O(10)-Y(2)-O(2)	172.15(8)	C(5)-C(4)-C(3)	119.0(4)
O(1)-Y(2)-O(5)	123.95(9)	C(5)-C(4)-H(4)	120.5
O(14)-Y(2)-O(5)	146.06(9)	C(3)-C(4)-H(4)	120.5
O(8)-Y(2)-O(5)	78.29(9)	C(10)-C(9)-C(8)	118.8(4)
O(11)-Y(2)-O(5)	91.39(9)	C(10)-C(9)-H(9)	120.6
O(13)-Y(2)-O(5)	142.23(9)	C(8)-C(9)-H(9)	120.6
O(4)-Y(2)-O(5)	52.04(8)	N(7)-C(8)-C(9)	120.8(3)
O(10)-Y(2)-O(5)	74.22(9)	N(7)-C(8)-C(7)	119.0(3)
O(2)-Y(2)-O(5)	108.13(9)	C(9)-C(8)-C(7)	120.1(3)
O(1)-Y(2)-O(7)	123.62(9)	C(2)-C(3)-C(4)	120.1(4)
O(14)-Y(2)-O(7)	118.38(8)	C(2)-C(3)-H(3)	120.0
O(8)-Y(2)-O(7)	52.23(8)	C(4)-C(3)-H(3)	120.0
O(11)-Y(2)-O(7)	163.39(9)	C(1)-C(2)-C(3)	119.2(4)
O(13)-Y(2)-O(7)	71.17(9)	C(1)-C(2)-H(2)	120.4
O(4)-Y(2)-O(7)	94.48(9)	C(3)-C(2)-H(2)	120.4
O(10)-Y(2)-O(7)	116.43(9)	N(7)-C(12)-C(11)	121.8(4)
O(2)-Y(2)-O(7)	71.30(9)	N(7)-C(12)-H(12)	119.1
O(5)-Y(2)-O(7)	72.74(9)	C(11)-C(12)-H(12)	119.1
O(1)-Y(2)-N(5)	80.35(9)	C(11)-C(10)-C(9)	120.3(4)
O(14)-Y(2)-N(5)	26.48(8)	C(11)-C(10)-H(10)	119.9
O(8)-Y(2)-N(5)	77.68(8)	C(9)-C(10)-H(10)	119.9
O(11)-Y(2)-N(5)	97.71(9)	C(12)-C(11)-C(10)	118.2(4)
O(13)-Y(2)-N(5)	26.01(8)	C(12)-C(11)-H(11)	120.9
O(4)-Y(2)-N(5)	151.97(8)	C(10)-C(11)-H(11)	120.9
O(10)-Y(2)-N(5)	93.63(9)	N(9)-C(17)-C(16)	119.6(3)
O(2)-Y(2)-N(5)	86.80(9)	N(9)-C(17)-C(18)	120.0(3)
O(5)-Y(2)-N(5)	155.69(8)	C(16)-C(17)-C(18)	120.4(3)
O(7)-Y(2)-N(5)	95.16(8)	N(11)-C(18)-C(19)	118.5(3)
O(1)-Y(2)-N(1)	26.20(9)	N(11)-C(18)-C(17)	111.1(3)
O(14)-Y(2)-N(1)	93.59(9)	C(19)-C(18)-C(17)	130.4(3)
O(8)-Y(2)-N(1)	142.21(9)	N(9)-C(13)-C(14)	121.0(3)

O(11)-Y(2)-N(1)	94.14(10)	N(9)-C(13)-H(13)	119.5
O(13)-Y(2)-N(1)	78.10(9)	C(14)-C(13)-H(13)	119.5
O(4)-Y(2)-N(1)	68.44(9)	C(16)-C(15)-C(14)	120.0(3)
O(10)-Y(2)-N(1)	145.97(9)	C(16)-C(15)-H(15)	120.0
O(2)-Y(2)-N(1)	26.26(9)	C(14)-C(15)-H(15)	120.0
O(5)-Y(2)-N(1)	117.68(9)	C(13)-C(14)-C(15)	118.7(3)
O(7)-Y(2)-N(1)	97.57(9)	C(13)-C(14)-H(14)	120.7
N(5)-Y(2)-N(1)	84.22(9)	C(15)-C(14)-H(14)	120.7
O(15)-N(5)-O(13)	122.3(3)	C(15)-C(16)-C(17)	119.2(3)
O(15)-N(5)-O(14)	122.4(3)	C(15)-C(16)-H(16)	120.4
O(13)-N(5)-O(14)	115.3(3)	C(17)-C(16)-H(16)	120.4
O(15)-N(5)-Y(2)	175.8(2)	C(24)-N(10)-C(20)	121.0(3)
O(13)-N(5)-Y(2)	57.93(16)	N(10)-C(20)-C(21)	119.7(3)
O(14)-N(5)-Y(2)	57.50(15)	N(10)-C(20)-C(19)	119.6(3)
O(6)-N(2)-O(5)	123.0(3)	C(21)-C(20)-C(19)	120.6(3)
O(6)-N(2)-O(4)	121.6(3)	C(22)-C(21)-C(20)	119.4(3)
O(5)-N(2)-O(4)	115.4(3)	C(22)-C(21)-H(21)	120.3
O(6)-N(2)-Y(2)	178.8(3)	C(20)-C(21)-H(21)	120.3
O(5)-N(2)-Y(2)	58.12(16)	C(21)-C(22)-C(23)	119.8(3)
O(4)-N(2)-Y(2)	57.28(16)	C(21)-C(22)-H(22)	120.1
N(4)-O(10)-Y(2)	95.7(2)	C(23)-C(22)-H(22)	120.1
N(1)-O(2)-Y(2)	95.1(2)	C(24)-C(23)-C(22)	118.5(3)
N(3)-O(8)-Y(2)	96.62(18)	C(24)-C(23)-H(23)	120.8
N(3)-O(7)-Y(2)	94.82(18)	C(22)-C(23)-H(23)	120.8
N(5)-O(14)-Y(2)	96.02(18)	N(10)-C(24)-C(23)	121.5(3)
N(2)-O(5)-Y(2)	96.12(19)	N(10)-C(24)-H(24)	119.2
N(4)-O(11)-Y(2)	96.27(19)	C(23)-C(24)-H(24)	119.2
N(2)-O(4)-Y(2)	96.43(19)	C(19)#2-N(11)-C(18)	123.3(3)
N(5)-O(13)-Y(2)	96.06(18)	N(11)#2-C(19)-C(18)	118.3(3)
O(9)-N(3)-O(7)	122.3(3)	N(11)#2-C(19)-C(20)	111.5(3)
O(9)-N(3)-O(8)	122.0(3)	C(18)-C(19)-C(20)	130.2(3)

Symmetrytransformationsusedtogenerateequivalentatoms: #1 -x+1, -y, -z+1; #2 -x+2, -y+1, -z.

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1-Eu**.

	x	y	z	U(eq)
H(1A)	7441	2257	1291	51
H(2A)	7804	3350	1918	44
H(3A)	6278	1784	4145	44
H(4A)	5648	1985	624	43
H(4B)	4425	3821	1066	38
H(9A)	2669	922	-1347	35
H(10A)	3795	10	-1825	39
H(12A)	6598	822	-233	39
H(11A)	5801	-27	-1281	41

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **1-Tb**.

	x	y	z	U(eq)
H(1)	7449	2258	1260	51
H(2)	7804	3352	1913	47
H(3)	6279	4152	1792	47
H(4)	4421	3819	1083	41
H(9)	35	-1337	915	2658
H(10)	3780	-2	-1825	39
H(11)	42	-1292	-45	5794
H(12)	6596	808	-252	40

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2-Er**.

	x	y	z	U(eq)
H(1A)	8388	6700	-737	54
H(2A)	7721	5511	-2587	55
H(3A)	5997	5845	-3482	50
H(4A)	4998	7412	-2509	40
H(15A)	5838	17190	4569	35
H(16A)	7493	16656	5367	31
H(9B)	5129	10373	2900	35

H(10B)	6060	10021	4373	41
H(11A)	7671	8933	4065	44
H(12A)	8282	8162	2291	42
H(13A)	35	1546	14938	6384
H(14A)	5295	16340	2636	38
H(21A)	9841	18051	6711	33
H(24A)	12036	17611	9609	41
H(22A)	10211	19595	8468	36
H(23A)	11279	19351	9954	41

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2-Y**.

	x	y	z	U(eq)
H(1)	1713	1829	2709	50
H(2)	2334	1058	927	52
H(3)	3958	-7	624	51
H(4)	4873	-380	2100	44
H(9)	5004	2595	7501	49
H(10)	3999	4141	8477	60
H(11)	2266	4482	7591	65
H(12)	1617	3300	5724	63
H(13)	6394	4947	-3445	42
H(14)	5299	6341	-2356	46
H(15)	5836	7184	-422	46
H(16)	40	372	6661	7500
H(21)	10150	1943	-1716	40
H(22)	9800	416	-3474	48
H(23)	8697	645	-4950	49
H(24)	7952	2392	-4609	49