

Electronic Supplementary Information

Fig. S1 IR spectra of the complexes 1 (a), 2 (b), 3 (c), 4 (d), 5 (e) and 6(f).



Fig. S2a-f PXRD patterns for the final residues of complexes **1-6** after thermal analyses [**1'-6'** are the experimental data, PXRD patterns of Tb_4O_7 , Eu_2O_3 and Sm_2O_3 are available in Powder Diffraction File (JCPDS NO. 32-1286, 34-0392 and 42-1461)].

Table S1. Crystal Data and Structure Refinements for Complexes 1-6

	Complex 1	Complex 2	Complex 3	Complex 4	Complex 5	Complex 6	
Formula	C40H22N9O7Tb	C46H26N9O6Eu	C46H26N9O6Sm	C ₂₄ H ₁₅ N ₄ O ₆ Eu	$C_{24}H_{15}N_4O_6Tb$	$C_{26}H_{19}N_4O_6Tb$	
Formula mass	899.58	952.72	951.11	607.36	614.32	642.37	
Crystal system	monoclinic	triclinic	triclinic	triclinic	triclinic	triclinic	
Space group	$P2_{1}/n$	Pī	Pī	Pī	Pī	Pī	
Crystal size (mm)	0.80 x 0.130 x 0.110	0.610 x 0.320 x 0.120	0.276 x 0.243 x 0.198	0.231 x 0.195 x 0.152	0.230 x 0.100 x 0.090	0.210 x 0.170 x 0.110	
a (Å)	12.2247(5)	10.5943(18)	10.6094(6)	9.434(4)	9.425(3)	9.6004(5)	

<i>b</i> (Å)	17.6302(7)	13.708(2)	13.7009(7)	9.625(3)	9.631(3)	11.0929(6)
<i>c</i> (Å)	16.1153(7)	14.497(2)	14.5285(7)	12.739(4)	12.716(3)	12.7617(7)
α (°)	90	78.663(3)	78.7380(10)	107.69(4)	107.168(4)	68.4090(10)
β (°)	98.1080(10)	80.397(3)	80.4200(10)	92.975(7)	93.018(5)	71.4530(10)
γ (°)	90	68.379(3)	68.3690(10)	100.613(9)	100.793(4)	74.6470(10)
$V(Å^3)$	3438.5(2)	1908.7(6)	1914.96(17)	1076.0(7)	1076.1(5)	1181.14(11)
Ζ	4	2	2	2	2	2
Goodness-of-fit on	1.017	1.067	1.030	1.019	1.044	1.059
F^2						
Reflns	18552 / 6715	10506 / 7380	10623 / 7452	7423/ 4743	5842 / 4184	6063 / 4281
collected/unique						
θ Range (°)	1.72 to 25.35	1.44 to 26.00	1.44 to 26.05	1.69 to 27.18	1.69 to 26.08	1.77 to 25.35
$R(I>2\sigma(I))$	$R_1 = 0.0316$ $wR_2 = 0.0630$	$R_1 = 0.0348$ $wR_2 = 0.0749$	$R_1 = 0.0391$ $wR_2 = 0.0768$	$R_1 = 0.0550$ $wR_2 = 0.0955$	$R_1 = 0.0509$ $wR_2 = 0.1121$	$R_1 = 0.0227$ $wR_2 = 0.0525$
R (all data)	$R_1 = 0.0493$	$R_1 = 0.0433$	$R_1 = 0.0511$	$R_1 = 0.0795$	$R_1 = 0.0654$	$R_1 = 0.0260$
	$wR_2 = 0.0694$	$wR_2 = 0.0789$	$wR_2 = 0.0824$	$wR_2 = 0.1069$	$wR_2 = 0.1213$	$wR_2 = 0.0543$

Table S2. Selected bond lengths and bond angles for 1-6

1		2		3		4		5		6	
Bond lengths	Å	Bond lengths	Å	Bond lengths	Å	Bond lengths	Å	Bond lengths	Å	Bond lengths	Å
Tb-O(1)#2		Eu-O(1)#1	2.664(3)	Sm-O(1)#1	2.477(3)	Eu-O(1)	2.412(5)	Tb-O(1)#3	2.363(5)	Tb-O(1)#6	2.377(2)
	2.506(3)										
Tb-O(2)#2	2.590(3)	Eu-O(2) ^{#1}	2.421(3)	Sm-O(2)#1	2.595(3)	Eu-O(2)#2	2.371(5)	Tb-O(2)	2.386(5)	Tb-O(2)#5	2.378(2)
Tb-O(3)#1	2.441(3)	Eu-O(3)#2	2.461(2)	Sm-O(3)#2	2.667(3)	Eu-O(3)	2.607(5)	Tb-O(3)	2.455(6)	Tb-O(3)	2.408(2)
Tb-O(4)#1	2.481(3)	Eu-O(4)#2	2.585(2)	Sm-O(4)#2	2.438(3)	Eu-O(4)	2.516(5)	Tb-O(4)	2.408(6)	Tb-O(3)#1	2.468(2)
Tb-O(5)	2.486(3)	Eu-O(5)	2.523(3)	Sm-O(5)	2.539(3)	Eu-O(5)#3	2.462(5)	Tb-O(5)#5	2.605(6)	Tb-O(4)#1	2.646(2)
Tb-O(6)	2.500(3)	Eu-O(6)	2.495(3)	Sm-O(6)	2.505(3)	Eu-O(4)#2	2.443(5)	Tb-O(6)#4	2.427(5)	Tb-O(5)	2.404(2)
Tb-N(1)	2.598(3)	Eu-N(1)	2.569(3)	Sm-N(1)	2.684(3)	Eu-O(6)#3	2.427(5)	Tb-O(6)#5	2.483(6)	Tb-O(6)	2.424(3)
Tb-N(2)	2.646(3)	Eu-N(2)	2.689(3)	Sm-N(2)	2.634(3)	Eu-N(1)#4	2.554(5)	Tb-N(3)#2	2.558(6)	Tb-N(1)	2.535(3)
Tb-N(5)	2.539(3)	Eu-N(5)	2.676(3)	Sm-N(5)	2.583(3)	Eu-N(2)#4	2.574(6)	Tb-N(4)#2	2.532(6)	Tb-N(2)	2.540(3)
Tb-N(6)	2.589(3)	Eu-N(6)	2.626(3)	Sm-N(6)	2.711(3)						

Bond angles	0	Bond angles	0	Bond angles	0	Bond angles	0	Bond angles	0	Bond angles	0
O(1)#2-Tb-N(5)	78.69(9)	O(1)#1-Eu-N(5)	75.12(9)	O(1)#1-Sm-N(5)	78.21(9)	O(2)#2-Eu-O(1)	139.11(17)	O(1)#3-Tb-O(2)	139.65(19)	O(1)#6-Tb-	139.87(8)
										O(2) ^{#5}	
O(3)#1-Tb-	105.03(8	O(2)#1-Eu-O(3)#2	112.12(9)	$O(2)^{\#_1}$ -Sm- $O(3)^{\#_2}$	67.22(9)	O(1)-Eu-O(3)	67.13(17)	O(1)#3-Tb-O(3)	110.8(2)	O(1)#6-Tb-	70.98(9)
O(2)#2)									O(3)	
O(4)#1-Tb-O(5)	74.73(9)	O(5)-Eu-O(4)#2	140.17(8)	O(4)#2-Sm-O(5)	95.00(10)	O(1)-Eu-O(6)#2	75.58(17)	O(1)#3-Tb-	70.62(19)	O(1)#6-Tb-	115.43(9)
								O(6)#4		O(6)	
O(5)-Tb-O(6)	50.77(9)	O(6)-Eu-O(5)	52.01(9)	O(6)-Sm-O(5)	51.80(10)	O(2)#2-Eu-O(4)	69.66(17)	O(2)-Tb-O(4)	133.13(19)	O(2)#5-Tb-	67.42(8)
										O(4)#1	
O(3)#1-Tb-N(5)	68.86(9)	O(3)#2-Eu-N(5)	68.44(9)	N(5)-Sm-O(3)#2	143.49(9)	O(3)-Eu-O(4)	50.45(14)	O(4)-Tb-O(3)	53.44(19)	O(3)-Tb-	119.12(7)
										O(4)#1	
O(5)-Tb-N(5)	144.92(1	O(5)-Eu-N(5)	103.86(9)	O(5)-Sm-N(5)	81.47(10)	O(3)-Eu-O(5)#3	137.59(17)	O(3)-Tb-O(5)#5	137.58(18)	O(5)-Tb-O(3)	96.04(9)
	0)										
O(6)-Tb-N(6)	74.43(10	O(6)-Eu-N(6)	76.27(9)	O(6)-Sm-N(6)	108.29(10	O(6)#2-Eu-O(3)	142.50(17)	O(6)#5-Tb-	50.83(17)	O(5)-Tb-O(6)	53.65(9)
))			O(5)#5			
N(5)-Tb-N(6)	64.46(10	N(6)-Eu-N(5)	61.97(9)	N(5)-Sm-N(6)	61.90(10)	O(3)-Eu-N(2)#4	70.03(17)	O(3)-Tb-N(3)#2	120.11(19)	O(3)-Tb-N(1)	148.01(9)
)										
N(1)-Tb-N(2)	62.16(9)	N(1)-Eu-N(2)	62.01(10)	N(2)-Sm-N(1)	61.62(10)	O(1)-Eu-N(1)#4	83.28(17)	O(1)#3-Tb-	137.25(19)	O(1)#6-Tb-	137.21(9)
								N(4)#2		N(2)	
N(1)-Tb-N(9)	85.54(11	N(1)-Eu-N(5)	112.80(10	N(5)-Sm-N(1)	113.07(10	N(1)#4-Eu-	64.12(19)	N(4)#2-Tb-	64.80(19)	N(1)-Tb-N(2)	64.81(9)
)))	N(2)#4		N(3)#2			

Symmetry transformations used to generate equivalent atoms: 1: #1 -x,-y+1,-z+2; #2 x-1/2,-y+1/2,z-1/2. 2: #1 -x+2,-y,-z+2; #2 -x+1,-y+1,-z+1. 3: #1 -x+1,y,-z+2; #2 -x,-y+1,-z+1. 4: #2 -x+2,-y+2,-z+2; #3 x+1,y,z; #4 -x+2,-y+2,-z+1. 5: #2 -x+2,-y+1,-z+1; #3 -x+2,-y+1,-z; #4 -x+1,-y+1,-z; #5 x+1,y,z. 6: #1 x+2,-y,-z+2; #5 -x+2,-y,-z+1; #6 x,y,z+1.