Electronic Supplementary Material (ESI) for Dalton Transactions.

Heterometallic Trinuclear $\{Co^{III}_2Ln^{III}\}$ (Ln = Gd, Tb Ho and Er) Complexes in a Bent Geometry. Field-induced Single-Ion Magnet Behavior of the Er^{III} and Tb^{III} Analogues

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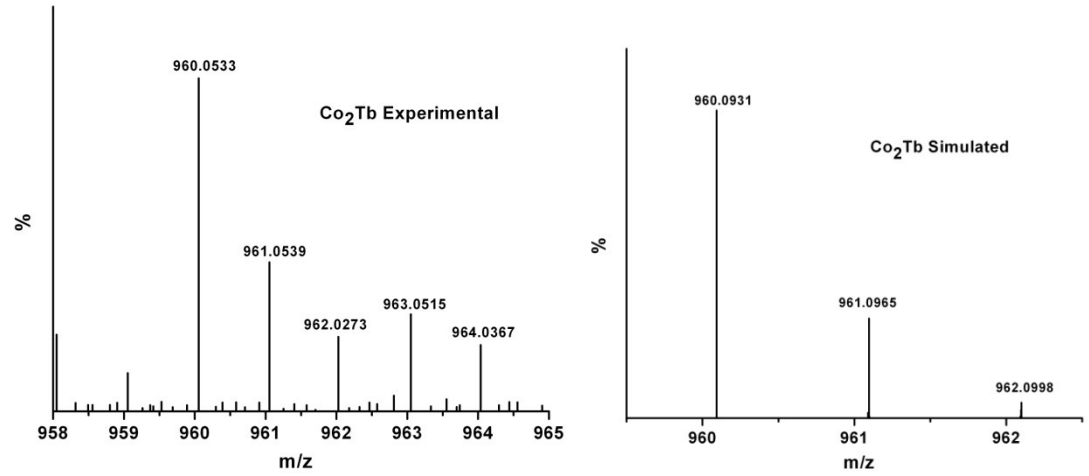
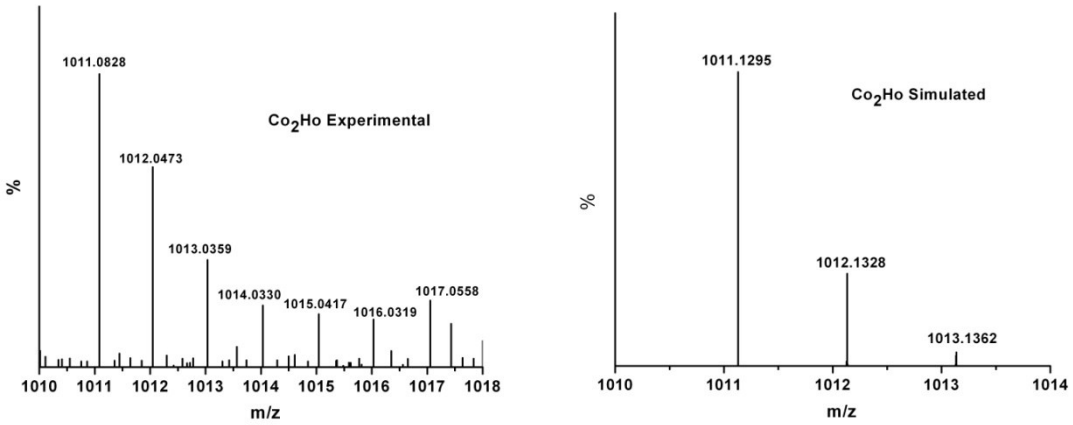


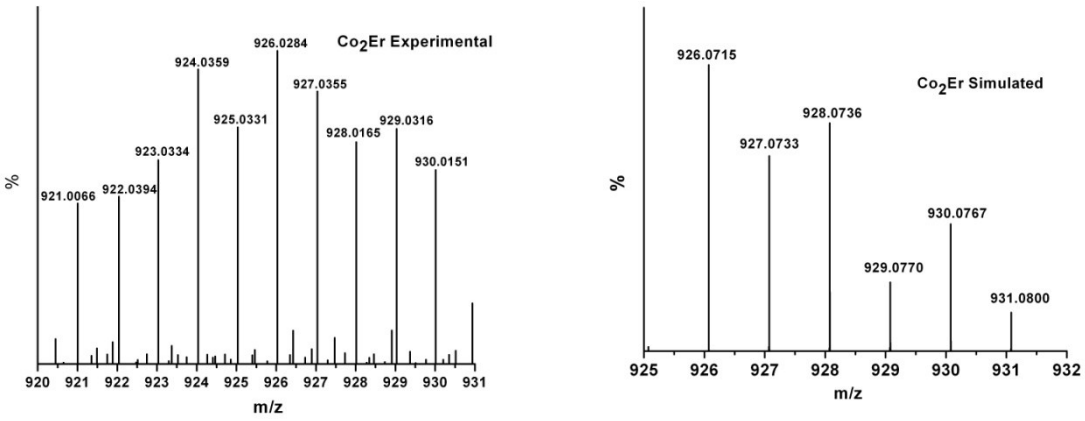
(a) (b)

Figure S1. (a)ESI-MS spectrum of complex **2** (Experimental) and (b) Simulated isotopic pattern for the parent ion peak of **2**



(a) (b)

Figure S2. (a) ESI-MS spectrum of complex **3**(Experimental) and (b) Simulated isotopic pattern for the parent ion peak of **3**



(a) (b)

Figure S3. (a)ESI-MS spectrum of complex **4**(Experimental) and (b) Simulated isotopic pattern for the parent ion peak of **4**

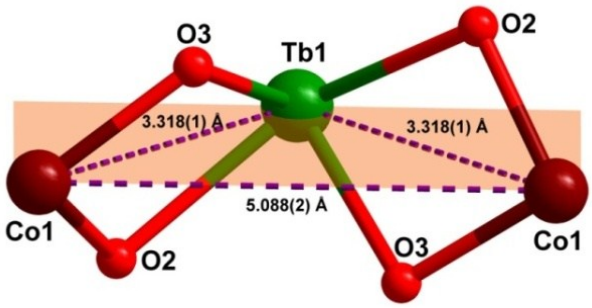


Figure S4. Mean planes of **2**. Isosceles triangular arrangement of the metal ions.

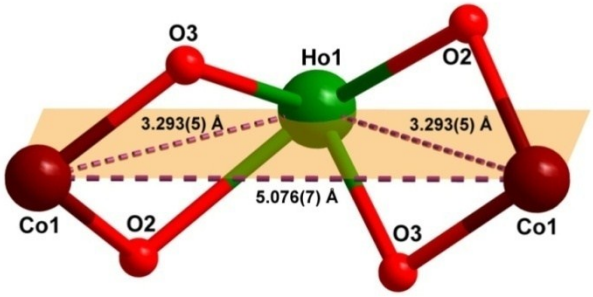


Figure S5. Mean planes of **3**. Isosceles triangular arrangement of the metal ions.

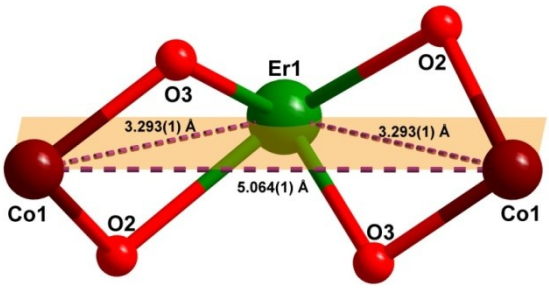


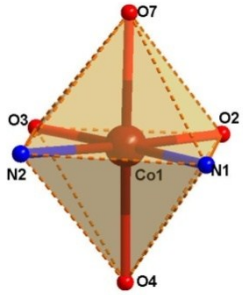
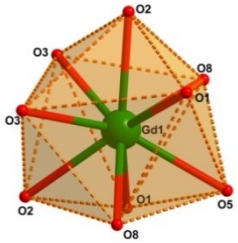
Figure S6. Mean planes of **4**. Isosceles triangular arrangement of the metal ions.

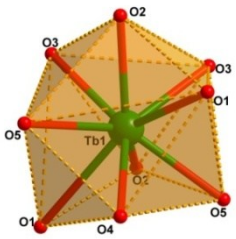
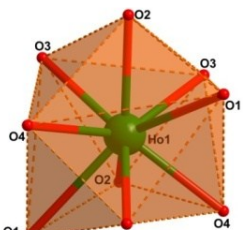
Table S1. Bond valence sum (BVS) calculations of Co oxidation state in compounds **1-4**

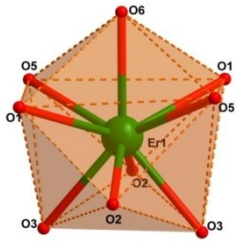
Compounds	Bond distances	Co^{2+} R_0 (1.692)	Co^{3+} R_0 (1.680)	Assigned
1	Co-N(1) = 1.875(3)	0.618	0.598	
	Co-N(2) = 1.903(3)	0.618	0.598	
	Co-O(2) = 1.878(2)	0.606	0.587	
	Co-O(3) = 1.898(3)	0.557	0.539	
	Co-O(5) = 1.923(3)	0.550	0.532	
	Co-O(6) = 1.941(4)	0.510	0.493	
		3.45	3.34	Co^{3+}
2	Co-N(1) = 1.869(8)	0.606	0.587	
	Co-N(2) = 1.920(7)	0.600	0.580	
	Co-O(2) = 1.892(5)	0.577	0.559	
	Co-O(3) = 1.888(5)	0.568	0.550	
	Co-O(4) = 1.933(6)	0.519	0.503	
	Co-O(6) = 1.959(7)	0.476	0.461	
		3.34	3.24	Co^{3+}
3	Co-N(1) = 1.875(4)	0.601	0.582	
	Co-N(2) = 1.913(4)	0.601	0.582	
	Co-O(2) = 1.872(3)	0.585	0.566	
	Co-O(3) = 1.887(3)	0.585	0.566	
	Co-O(4) = 1.918(3)	0.525	0.508	
	Co-O(6) = 1.955(4)	0.497	0.482	
		3.39	3.28	Co^{3+}
4	Co-N(1) = 1.880(4)	0.611	0.591	
	Co-N(2) = 1.905(4)	0.598	0.579	
	Co-O(2) = 1.881(3)	0.584	0.565	
	Co-O(3) = 1.898(3)	0.574	0.556	
	Co-O(5) = 1.923(4)	0.538	0.521	
	Co-O(4) = 1.944(5)	0.534	0.517	

		3.43	3.32	Co^{3+}

Table S2. Coordination geometry around the lanthanide ions, bond distances (Å) and bond angles (°) of complexes **1-4**

Coordination Geometry	Bond Distances (Å)	Bond Angles (°)
 Complex **1**: Distorted octahedral	Co(1)-N(1) 1.870(8) Co(1)-N(2) 1.87(2) Co(1)-O(2) 1.877(6) Co(1)-O(3) 1.908(7) Co(1)-O(7) 1.913(7) Co(1)-O(6) 1.941(10)	N(1)-Co(1)-N(2) 86.9(6) N(1)-Co(1)-O(2) 96.7(3) N(2)-Co(1)-O(2) 176.4(6) N(1)-Co(1)-O(3) 174.8(3) N(2)-Co(1)-O(3) 88.1(6) O(2)-Co(1)-O(3) 88.4(3) N(1)-Co(1)-O(7) 87.9(3) N(2)-Co(1)-O(7) 86.4(7) O(2)-Co(1)-O(7) 93.1(3) O(3)-Co(1)-O(7) 92.9(3) N(1)-Co(1)-O(6) 91.4(4) N(2)-Co(1)-O(6) 93.6(7) O(2)-Co(1)-O(6) 86.9(4) O(3)-Co(1)-O(6) 87.8(4) O(7)-Co(1)-O(6) 179.3(4)
 Complex **1**: Distorted mono cappedsquare-antiprismatic	Gd(1)-O(8) 2.363(7) Gd(1)-O(8)#1 2.363(7) Gd(1)-O(2) 2.385(6) Gd(1)-O(2)#1 2.385(6) Gd(1)-O(3) 2.391(7) Gd(1)-O(3)#1 2.391(7) Gd(1)-O(5) 2.394(12) Gd(1)-O(1)#1 2.689(7) Gd(1)-O(1) 2.689(7)	O(8)-Gd(1)-O(8)#1 135.9(4) O(8)-Gd(1)-O(2) 73.9(2) O(8)#1-Gd(1)-O(2) 126.1(2) O(8)-Gd(1)-O(2)#1 126.1(2) O(8)#1-Gd(1)-O(2)#1 73.9(2) O(2)-Gd(1)-O(2)#1 130.7(3) O(8)-Gd(1)-O(3) 75.2(3) O(8)#1-Gd(1)-O(3) 146.2(2) O(2)-Gd(1)-O(3) 67.0(2) O(2)#1-Gd(1)-O(3) 75.5(2) O(8)-Gd(1)-O(3)#1 146.2(2) O(8)#1-Gd(1)-O(3)#1 75.2(3) O(2)-Gd(1)-O(3)#1 75.5(2) O(2)#1-Gd(1)-O(3)#1 67.0(2) O(3)-Gd(1)-O(3)#1 79.8(4) O(8)-Gd(1)-O(5) 67.96(19) O(8)#1-Gd(1)-O(5) 68.0(2) O(2)-Gd(1)-O(5) 114.65(16) O(2)#1-Gd(1)-O(5) 114.64(16) O(3)-Gd(1)-O(5) 140.12(18) O(3)#1-Gd(1)-O(5) 140.11(18) O(8)-Gd(1)-O(1)#1 73.0(2) O(8)#1-Gd(1)-O(1)#1 93.8(3) O(2)-Gd(1)-O(1)#1 139.7(2) O(2)#1-Gd(1)-O(1)#1 59.1(2) O(3)-Gd(1)-O(1)#1 82.7(2) O(3)#1-Gd(1)-O(1)#1

		126.0(2) O(5)-Gd(1)-O(1)#1 72.54(16) O(8)-Gd(1)-O(1) 93.8(3) O(8)#1-Gd(1)-O(1) 73.0(2) O(2)-Gd(1)-O(1) 59.1(2) O(2)#1-Gd(1)-O(1) 139.7(2) O(3)-Gd(1)-O(1) 126.0(2) O(3)#1-Gd(1)-O(1) 82.7(2) O(5)-Gd(1)-O(1) 72.54(16) O(1)#1-Gd(1)-O(1) 145.1(3)
 Complex **2**: Distorted mono cappedsquare-antiprismatic	Tb(1)-O(5) 2.344(8) Tb(1)-O(5)#1 2.344(8) Tb(1)-O(4) 2.361(13) Tb(1)-O(2)#1 2.365(7) Tb(1)-O(2) 2.365(7) Tb(1)-O(3)#1 2.377(7) Tb(1)-O(3) 2.377(7) Tb(1)-O(1) 2.694(7) Tb(1)-O(1)#1 2.694(7)	O(5)-Tb(1)-O(5)#1 135.4(4) O(5)-Tb(1)-O(4) 67.7(2) O(5)#1-Tb(1)-O(4) 67.7(2) O(5)-Tb(1)-O(2)#1 126.2(3) O(5)#1-Tb(1)-O(2)#1 73.8(3) O(4)-Tb(1)-O(2)#1 114.23(17) O(5)-Tb(1)-O(2) 73.8(3) O(5)#1-Tb(1)-O(2) 126.2(3) O(4)-Tb(1)-O(2) 114.23(17) O(2)#1-Tb(1)-O(2) 131.5(3) O(5)-Tb(1)-O(3)#1 146.7(3) O(5)#1-Tb(1)-O(3)#1 75.3(3) O(4)-Tb(1)-O(3)#1 140.07(17) O(2)#1-Tb(1)-O(3)#1 66.8(2) O(2)-Tb(1)-O(3)#1 76.3(2) O(5)-Tb(1)-O(3) 75.3(3) O(5)#1-Tb(1)-O(3) 146.7(3) O(4)-Tb(1)-O(3) 140.07(17) O(2)#1-Tb(1)-O(3) 76.3(2) O(2)-Tb(1)-O(3) 66.8(2) O(3)#1-Tb(1)-O(3) 79.9(3) O(5)-Tb(1)-O(1) 94.0(3) O(5)#1-Tb(1)-O(1) 72.3(3) O(4)-Tb(1)-O(1) 72.04(19) O(2)#1-Tb(1)-O(1) 139.3(2) O(2)-Tb(1)-O(1) 59.7(2) O(3)#1-Tb(1)-O(1) 83.2(3) O(3)-Tb(1)-O(1) 126.3(2) O(5)-Tb(1)-O(1)#1 72.3(3) O(5)#1-Tb(1)-O(1)#1 94.0(3) O(4)-Tb(1)-O(1)#1 72.04(19) O(2)#1-Tb(1)-O(1)#1 59.7(2) O(2)-Tb(1)-O(1)#1 139.2(2) O(3)#1-Tb(1)-O(1)#1 126.3(2) O(3)-Tb(1)-O(1)#1 83.2(3) O(1)-Tb(1)-O(1)#1 144.1(4)
	Ho(1)-O(4)#1 2.31(3)	O(4)#1-Ho(1)-O(4) 134.7(18)

Complex **3**: Distorted mono cappedsquare-antiprismatic	Ho(1)-O(4) 2.31(3) Ho(1)-O(2)#1 2.35(2) Ho(1)-O(2) 2.35(2) Ho(1)-O(3)#1 2.35(3) Ho(1)-O(3) 2.35(3) Ho(1)-O(6) 2.37(6) Ho(1)-O(1)#1 2.70(3) Ho(1)-O(1) 2.70(3)	O(4)#1-Ho(1)-O(2)#1 74.7(10) O(4)-Ho(1)-O(2)#1 125.2(11) O(4)#1-Ho(1)-O(2) 125.2(11) O(4)-Ho(1)-O(2) 74.7(10) O(2)#1-Ho(1)-O(2) 132.3(13) O(4)#1-Ho(1)-O(3)#1 75.5(11) O(4)-Ho(1)-O(3)#1 147.3(10) O(2)#1-Ho(1)-O(3)#1 67.5(8) O(2)-Ho(1)-O(3)#1 76.3(9) O(4)#1-Ho(1)-O(3) 147.3(10) O(4)-Ho(1)-O(3) 75.5(11) O(2)#1-Ho(1)-O(3) 76.3(9) O(2)-Ho(1)-O(3) 67.5(8) O(3)#1-Ho(1)-O(3) 80.0(14) O(4)#1-Ho(1)-O(6) 67.3(9) O(4)-Ho(1)-O(6) 67.3(9) O(2)#1-Ho(1)-O(6) 113.8(6) O(2)-Ho(1)-O(6) 113.8(6) O(3)#1-Ho(1)-O(6) 140.0(7) O(3)-Ho(1)-O(6) 140.0(7) O(4)#1-Ho(1)-O(1)#1 94.3(12) O(4)-Ho(1)-O(1)#1 71.7(10) O(2)#1-Ho(1)-O(1)#1 59.1(8) O(2)-Ho(1)-O(1)#1 139.8(9) O(3)#1-Ho(1)-O(1)#1 126.4(9) O(3)-Ho(1)-O(1)#1 83.2(10) O(6)-Ho(1)-O(1)#1 71.9(7) O(4)#1-Ho(1)-O(1) 71.7(10) O(4)-Ho(1)-O(1) 94.3(12) O(2)#1-Ho(1)-O(1) 139.8(9) O(2)-Ho(1)-O(1) 59.1(8) O(3)#1-Ho(1)-O(1) 83.2(10) O(3)-Ho(1)-O(1) 126.4(9) O(6)-Ho(1)-O(1) 71.9(7) O(1)#1-Ho(1)-O(1) 143.9(15)
 Complex **4**: Distorted mono cappedsquare-antiprismatic	Er(1)-O(5)#1 2.315(5) Er(1)-O(5) 2.315(5) Er(1)-O(3)#1 2.339(6) Er(1)-O(3) 2.339(6) Er(1)-O(2)#1 2.351(4) Er(1)-O(2) 2.351(4) Er(1)-O(6) 2.364(10) Er(1)-O(1)#1 2.702(5) Er(1)-O(1) 2.702(5)	O(5)#1-Er(1)-O(5) 134.0(3) O(5)#1-Er(1)-O(3)#1 75.7(2) O(5)-Er(1)-O(3)#1 147.5(2) O(5)#1-Er(1)-O(3) 147.5(2) O(5)-Er(1)-O(3) 75.7(2) O(3)#1-Er(1)-O(3) 80.7(3) O(5)#1-Er(1)-O(2)#1 74.55(18) O(5)-Er(1)-O(2)#1 126.00(19) O(3)#1-Er(1)-O(2)#1

		67.40(17) O(3)-Er(1)-O(2)#1 75.98(18) O(5)#1-Er(1)-O(2) 126.00(19) O(5)-Er(1)-O(2) 74.55(18) O(3)#1-Er(1)-O(2) 75.98(18) O(3)-Er(1)-O(2) 67.40(18) O(2)#1-Er(1)-O(2) 131.5(2) O(5)#1-Er(1)-O(6) 66.98(14) O(5)-Er(1)-O(6) 66.98(14) O(3)#1-Er(1)-O(6) 139.68(17) O(3)-Er(1)-O(6) 139.67(17) O(2)#1-Er(1)-O(6) 114.26(11) O(2)-Er(1)-O(6) 114.26(11) O(5)#1-Er(1)-O(1)#1 94.4(2) O(5)-Er(1)-O(1)#1 71.60(18) O(3)#1-Er(1)-O(1)#1 126.88(17) O(3)-Er(1)-O(1)#1 82.2(2) O(2)#1-Er(1)-O(1)#1 59.73(15) O(2)-Er(1)-O(1)#1 138.98(16) O(6)-Er(1)-O(1)#1 72.25(12) O(5)#1-Er(1)-O(1) 71.60(18) O(5)-Er(1)-O(1) 94.4(2) O(3)#1-Er(1)-O(1) 82.2(2) O(3)-Er(1)-O(1) 126.88(18) O(2)#1-Er(1)-O(1) 138.98(16) O(2)-Er(1)-O(1) 59.73(15) O(6)-Er(1)-O(1) 72.25(12) O(1)#1-Er(1)-O(1) 144.5(2)

Table S3. Selected bond lengths (Å) and bond angles (°) of the complexes **1-4.**

Complex 1:

Gd(1)-O(4)	2.360(3)	Gd(1)-O(4)#1	2.360(3)	Gd(1)-O(2)	2.385(2)
Gd(1)-O(2)#1	2.385(2)	Gd(1)-O(3)#1	2.389(3)	Gd(1)-O(3)	2.389(3)
Gd(1)-O(7)	2.398(5)	Gd(1)-O(1)#1	2.687(3)	Gd(1)-O(1)	2.687(3)
Gd(1)-Co(1)#1	3.3265(9)	Gd(1)-Co(1)	3.3265(9)	Co(1)-O(2)	1.878(2)
Co(1)-N(1)	1.875(3)	Co(1)-O(3)	1.898(3)	Co(1)-N(2)	1.903(3)
Co(1)-O(5)	1.923(3)	Co(1)-O(6)	1.941(4)		

O(4)-Gd(1)-O(4)#1	136.34(16)	O(4)-Gd(1)-O(2)	73.86(10)
O(4)#1-Gd(1)-O(2)	126.01(10)	O(4)-Gd(1)-O(2)#1	126.01(10)
O(4)#1-Gd(1)-O(2)#1	73.86(10)	O(2)-Gd(1)-O(2)#1	130.75(12)
O(4)-Gd(1)-O(3)#1	146.21(10)	O(4)#1-Gd(1)-O(3)#1	74.91(11)

O(2)-Gd(1)-O(3)#1	75.80(9)	O(2)#1-Gd(1)-O(3)#1	66.79(9)
O(4)-Gd(1)-O(3)	74.91(11)	O(4)#1-Gd(1)-O(3)	146.21(10)
O(2)-Gd(1)-O(3)	66.79(9)	O(2)#1-Gd(1)-O(3)	75.80(9)
O(3)#1-Gd(1)-O(3)	79.76(14)	O(4)-Gd(1)-O(7)	68.17(8)
O(4)#1-Gd(1)-O(7)	68.17(8)	O(2)-Gd(1)-O(7)	114.62(6)
O(2)#1-Gd(1)-O(7)	114.62(6)	O(3)#1-Gd(1)-O(7)	140.12(7)
O(3)-Gd(1)-O(7)	140.12(7)	O(4)-Gd(1)-O(1)#1	72.91(9)
O(4)#1-Gd(1)-O(1)#1	93.91(10)	O(2)-Gd(1)-O(1)#1	139.75(9)
O(2)#1-Gd(1)-O(1)#1	59.32(8)	O(3)#1-Gd(1)-O(1)#1	125.90(9)
O(3)-Gd(1)-O(1)#1	83.07(10)	O(7)-Gd(1)-O(1)#1	72.33(7)
O(4)-Gd(1)-O(1)	93.91(10)	O(4)#1-Gd(1)-O(1)	72.91(9)
O(2)-Gd(1)-O(1)	59.31(8)	O(2)#1-Gd(1)-O(1)	139.75(9)
O(3)#1-Gd(1)-O(1)	83.07(10)	O(3)-Gd(1)-O(1)	125.90(9)
O(7)-Gd(1)-O(1)	72.33(7)	O(1)#1-Gd(1)-O(1)	144.66(13)
O(4)-Gd(1)-Co(1)#1	152.93(9)	O(4)#1-Gd(1)-Co(1)#1	65.72(8)
O(2)-Gd(1)-Co(1)#1	107.25(7)	O(2)#1-Gd(1)-Co(1)#1	33.53(6)
O(3)#1-Gd(1)-Co(1)#1	34.04(6)	O(3)-Gd(1)-Co(1)#1	80.76(7)
O(7)-Gd(1)-Co(1)#1	130.130(16)	O(1)#1-Gd(1)-Co(1)#1	92.75(6)
O(1)-Gd(1)-Co(1)#1	110.08(7)	O(4)-Gd(1)-Co(1)	65.72(8)
O(4)#1-Gd(1)-Co(1)	152.93(9)	O(2)-Gd(1)-Co(1)	33.53(6)
O(2)#1-Gd(1)-Co(1)	107.25(7)	O(3)#1-Gd(1)-Co(1)	80.76(7)
O(3)-Gd(1)-Co(1)	34.04(6)	O(7)-Gd(1)-Co(1)	130.129(17)
O(1)#1-Gd(1)-Co(1)	110.08(7)	O(1)-Gd(1)-Co(1)	92.74(6)
Co(1)#1-Gd(1)-Co(1)	99.74(3)	O(2)-Co(1)-N(1)	96.44(13)
O(2)-Co(1)-O(3)	88.17(11)	N(1)-Co(1)-O(3)	175.36(14)
O(2)-Co(1)-N(2)	176.37(15)	N(1)-Co(1)-N(2)	86.95(16)
O(3)-Co(1)-N(2)	88.45(15)	O(2)-Co(1)-O(5)	93.11(12)
N(1)-Co(1)-O(5)	87.30(14)	O(3)-Co(1)-O(5)	92.98(12)
N(2)-Co(1)-O(5)	85.74(16)	O(2)-Co(1)-O(6)	87.16(15)
N(1)-Co(1)-O(6)	91.43(18)	O(3)-Co(1)-O(6)	88.27(16)
N(2)-Co(1)-O(6)	94.07(18)	O(5)-Co(1)-O(6)	178.72(16)
O(2)-Co(1)-Gd(1)	44.54(7)	N(1)-Co(1)-Gd(1)	139.83(11)
O(3)-Co(1)-Gd(1)	44.79(8)	N(2)-Co(1)-Gd(1)	131.88(13)
O(5)-Co(1)-Gd(1)	86.20(9)	O(6)-Co(1)-Gd(1)	94.86(12)
C(7)-O(2)-Co(1)	124.1(2)	C(7)-O(2)-Gd(1)	129.8(2)
Co(1)-O(2)-Gd(1)	101.92(10)	C(12)-O(3)-Co(1)	109.8(2)
C(12)-O(3)-Gd(1)	140.3(3)	Co(1)-O(3)-Gd(1)	101.17(11)
C(13)-O(5)-Co(1)	126.4(3)	C(2)-O(1)-C(1)	115.1(3)

C(2)-O(1)-Gd(1)	118.0(2)	C(1)-O(1)-Gd(1)	125.4(3)
C(13)-O(4)-Gd(1)	135.2(3)	C(8)-N(1)-C(9)	121.5(4)
C(8)-N(1)-Co(1)	125.9(3)	C(9)-N(1)-Co(1)	112.5(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z+3/2

Complex 2:

Tb(1)-O(5)	2.334(6)	Tb(1)-O(5)#1	2.334(6)	Tb(1)-O(2)#1	2.374(6)
Tb(1)-O(2)	2.374(6)	Tb(1)-O(3)#1	2.370(6)	Tb(1)-O(3)	2.370(6)
Tb(1)-O(7)	2.383(9)	Tb(1)-O(1)	2.699(6)	Tb(1)-O(1)#1	2.699(6)
Tb(1)-Co(1)	3.3184(13)	Tb(1)-Co(1)#1	3.3185(13)	Co(1)-O(3)	1.888(7)
Co(1)-N(1)	1.869(8)	Co(1)-O(2)	1.888(5)	Co(1)-N(2)	1.920(7)
Co(1)-O(4)	1.933(6)	Co(1)-O(6)	1.959(7)		

O(5)-Tb(1)-O(5)#1	135.1(3)	O(5)-Tb(1)-O(2)#1	125.6(2)
O(5)#1-Tb(1)-O(2)#1	74.4(2)	O(5)-Tb(1)-O(2)	74.4(2)
O(5)#1-Tb(1)-O(2)	125.6(2)	O(2)#1-Tb(1)-O(2)	131.4(3)
O(5)-Tb(1)-O(3)#1	146.9(2)	O(5)#1-Tb(1)-O(3)#1	75.6(2)
O(2)#1-Tb(1)-O(3)#1	66.8(2)	O(2)-Tb(1)-O(3)#1	76.1(2)
O(5)-Tb(1)-O(3)	75.6(2)	O(5)#1-Tb(1)-O(3)	146.9(2)
O(2)#1-Tb(1)-O(3)	76.1(2)	O(2)-Tb(1)-O(3)	66.8(2)
O(3)#1-Tb(1)-O(3)	79.2(3)	O(5)-Tb(1)-O(7)	67.56(17)
O(5)#1-Tb(1)-O(7)	67.56(17)	O(2)#1-Tb(1)-O(7)	114.28(13)
O(2)-Tb(1)-O(7)	114.28(13)	O(3)#1-Tb(1)-O(7)	140.40(16)
O(3)-Tb(1)-O(7)	140.40(16)	O(5)-Tb(1)-O(1)	94.0(2)
O(5)#1-Tb(1)-O(1)	72.2(2)	O(2)#1-Tb(1)-O(1)	139.84(18)
O(2)-Tb(1)-O(1)	59.28(18)	O(3)#1-Tb(1)-O(1)	83.6(2)
O(3)-Tb(1)-O(1)	125.9(2)	O(7)-Tb(1)-O(1)	72.05(14)
O(5)-Tb(1)-O(1)#1	72.2(2)	O(5)#1-Tb(1)-O(1)#1	94.0(2)
O(2)#1-Tb(1)-O(1)#1	59.28(18)	O(2)-Tb(1)-O(1)#1	139.84(18)
O(3)#1-Tb(1)-O(1)#1	125.9(2)	O(3)-Tb(1)-O(1)#1	83.6(2)
O(7)-Tb(1)-O(1)#1	72.05(14)	O(1)-Tb(1)-O(1)#1	144.1(3)
O(5)-Tb(1)-Co(1)	66.24(16)	O(5)#1-Tb(1)-Co(1)	153.28(18)
O(2)#1-Tb(1)-Co(1)	107.59(14)	O(2)-Tb(1)-Co(1)	33.86(13)
O(3)#1-Tb(1)-Co(1)	80.84(16)	O(3)-Tb(1)-Co(1)	33.83(16)
O(7)-Tb(1)-Co(1)	129.96(2)	O(1)-Tb(1)-Co(1)	93.03(13)

O(1)#1-Tb(1)-Co(1)	110.06(14)	O(5)-Tb(1)-Co(1)#1	153.28(18)
O(5)#1-Tb(1)-Co(1)#1	66.23(16)	O(2)#1-Tb(1)-Co(1)#1	33.86(13)
O(2)-Tb(1)-Co(1)#1	107.59(14)	O(3)#1-Tb(1)-Co(1)#1	33.83(16)
O(3)-Tb(1)-Co(1)#1	80.84(16)	O(7)-Tb(1)-Co(1)#1	129.96(2)
O(1)-Tb(1)-Co(1)#1	110.06(14)	O(1)#1-Tb(1)-Co(1)#1	93.03(13)
Co(1)-Tb(1)-Co(1)#1	100.08(5)	O(3)-Co(1)-N(1)	175.4(3)
O(3)-Co(1)-O(2)	87.6(3)	N(1)-Co(1)-O(2)	96.9(3)
O(3)-Co(1)-N(2)	88.7(3)	N(1)-Co(1)-N(2)	86.9(4)
O(2)-Co(1)-N(2)	176.1(3)	O(3)-Co(1)-O(4)	93.0(3)
N(1)-Co(1)-O(4)	87.8(3)	O(2)-Co(1)-O(4)	93.3(2)
N(2)-Co(1)-O(4)	85.9(3)	O(3)-Co(1)-O(6)	87.4(3)
N(1)-Co(1)-O(6)	91.8(3)	O(2)-Co(1)-O(6)	85.9(3)
N(2)-Co(1)-O(6)	94.9(3)	O(4)-Co(1)-O(6)	179.1(3)
O(3)-Co(1)-Tb(1)	44.34(19)	N(1)-Co(1)-Tb(1)	140.2(2)
O(2)-Co(1)-Tb(1)	44.48(18)	N(2)-Co(1)-Tb(1)	131.7(3)
O(4)-Co(1)-Tb(1)	86.12(18)	O(6)-Co(1)-Tb(1)	93.7(2)
C(12)-O(3)-Co(1)	109.7(5)	C(12)-O(3)-Tb(1)	139.0(6)
Co(1)-O(3)-Tb(1)	101.8(3)	C(7)-O(2)-Co(1)	123.8(5)
C(7)-O(2)-Tb(1)	130.2(5)	Co(1)-O(2)-Tb(1)	101.7(2)
C(13)-O(4)-Co(1)	125.8(6)	C(2)-O(1)-C(1)	114.4(7)
C(2)-O(1)-Tb(1)	118.1(5)	C(1)-O(1)-Tb(1)	126.1(6)
C(13)-O(5)-Tb(1)	134.4(6)	C(8)-N(1)-C(9)	122.4(8)
C(8)-N(1)-Co(1)	124.3(7)	C(9)-N(1)-Co(1)	113.1(6)
C(1B)-N(2)-C(2B)	122.0(12)	C(1A)-N(2)-C(2A)	117.3(12)
C(1B)-N(2)-Co(1)	110.8(8)	C(2B)-N(2)-Co(1)	109.9(9)
C(1A)-N(2)-Co(1)	106.1(9)	C(2A)-N(2)-Co(1)	108.7(8)

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

Complex 3:

Ho(1)-O(5)	2.316(3)	Ho(1)-O(5)#1	2.316(3)	Ho(1)-O(2)#1	2.352(2)
Ho(1)-O(2)	2.352(2)	Ho(1)-O(3)	2.353(3)	Ho(1)-O(3)#1	2.353(3)
Ho(1)-O(7)	2.388(6)	Ho(1)-O(1)	2.700(3)	Ho(1)-O(1)#1	2.700(3)
Ho(1)-Co(1)	3.2923(9)	Ho(1)-Co(1)#1	3.2923(9)	Co(1)-O(2)	1.872(3)
Co(1)-N(1)	1.875(4)	Co(1)-O(3)	1.887(3)	Co(1)-N(2)	1.913(4)
Co(1)-O(4)	1.918(3)	Co(1)-O(6)	1.955(4)		

O(5)-Ho(1)-O(5)#1	134.78(19)	O(5)-Ho(1)-O(2)#1	125.18(12)

O(5)#1-Ho(1)-O(2)#1	74.64(11)	O(5)-Ho(1)-O(2)	74.64(11)
O(5)#1-Ho(1)-O(2)	125.18(12)	O(2)#1-Ho(1)-O(2)	132.25(13)
O(5)-Ho(1)-O(3)	75.37(12)	O(5)#1-Ho(1)-O(3)	147.41(11)
O(2)#1-Ho(1)-O(3)	76.49(9)	O(2)-Ho(1)-O(3)	67.20(9)
O(5)-Ho(1)-O(3)#1	147.41(11)	O(5)#1-Ho(1)-O(3)#1	75.37(12)
O(2)#1-Ho(1)-O(3)#1	67.20(9)	O(2)-Ho(1)-O(3)#1	76.49(9)
O(3)-Ho(1)-O(3)#1	79.78(14)	O(5)-Ho(1)-O(7)	67.39(9)
O(5)#1-Ho(1)-O(7)	67.39(9)	O(2)#1-Ho(1)-O(7)	113.88(7)
O(2)-Ho(1)-O(7)	113.88(7)	O(3)-Ho(1)-O(7)	140.11(7)
O(3)#1-Ho(1)-O(7)	140.11(7)	O(5)-Ho(1)-O(1)	94.44(12)
O(5)#1-Ho(1)-O(1)	71.49(11)	O(2)#1-Ho(1)-O(1)	139.71(9)
O(2)-Ho(1)-O(1)	59.33(9)	O(3)-Ho(1)-O(1)	126.31(9)
O(3)#1-Ho(1)-O(1)	83.51(11)	O(7)-Ho(1)-O(1)	71.81(8)
O(5)-Ho(1)-O(1)#1	71.49(11)	O(5)#1-Ho(1)-O(1)#1	94.45(12)
O(2)#1-Ho(1)-O(1)#1	59.33(9)	O(2)-Ho(1)-O(1)#1	139.71(9)
O(3)-Ho(1)-O(1)#1	83.51(11)	O(3)#1-Ho(1)-O(1)#1	126.30(9)
O(7)-Ho(1)-O(1)#1	71.81(8)	O(1)-Ho(1)-O(1)#1	143.62(16)
O(5)-Ho(1)-Co(1)	66.26(9)	O(5)#1-Ho(1)-Co(1)	153.18(10)
O(2)#1-Ho(1)-Co(1)	108.36(7)	O(2)-Ho(1)-Co(1)	33.82(6)
O(3)-Ho(1)-Co(1)	34.21(6)	O(3)#1-Ho(1)-Co(1)	81.34(7)
O(7)-Ho(1)-Co(1)	129.575(16)	O(1)-Ho(1)-Co(1)	93.05(7)
O(1)#1-Ho(1)-Co(1)	110.15(8)	O(5)-Ho(1)-Co(1)#1	153.19(10)
O(5)#1-Ho(1)-Co(1)#1	66.26(9)	O(2)#1-Ho(1)-Co(1)#1	33.83(6)
O(2)-Ho(1)-Co(1)#1	108.36(7)	O(3)-Ho(1)-Co(1)#1	81.34(7)
O(3)#1-Ho(1)-Co(1)#1	34.21(6)	O(7)-Ho(1)-Co(1)#1	129.575(17)
O(1)-Ho(1)-Co(1)#1	110.15(8)	O(1)#1-Ho(1)-Co(1)#1	93.05(7)
Co(1)-Ho(1)-Co(1)#1	100.85(3)	O(2)-Co(1)-N(1)	97.13(14)
O(2)-Co(1)-O(3)	87.67(11)	N(1)-Co(1)-O(3)	175.12(14)
O(2)-Co(1)-N(2)	175.90(16)	N(1)-Co(1)-N(2)	86.70(18)
O(3)-Co(1)-N(2)	88.53(16)	O(2)-Co(1)-O(4)	92.66(13)
N(1)-Co(1)-O(4)	87.38(15)	O(3)-Co(1)-O(4)	93.30(12)
N(2)-Co(1)-O(4)	86.03(19)	O(2)-Co(1)-O(6)	87.09(15)
N(1)-Co(1)-O(6)	91.29(18)	O(3)-Co(1)-O(6)	88.06(15)
N(2)-Co(1)-O(6)	94.3(2)	O(4)-Co(1)-O(6)	178.60(16)
O(2)-Co(1)-Ho(1)	44.387)	N(1)-Co(1)-Ho(1)	140.39(12)
O(3)-Co(1)-Ho(1)	44.49(8)	N(2)-Co(1)-Ho(1)	131.58(14)
O(4)-Co(1)-Ho(1)	85.97(10)	O(6)-Co(1)-Ho(1)	94.80(12)
C(8)-N(1)-Co(1)	124.7(3)	C(9)-N(1)-Co(1)	112.1(3)

C(1A)-N(2)-Co(1)	108.6(5)	C(1B)-N(2)-Co(1)	109.0(6)
C(2A)-N(2)-Co(1)	108.4(5)	C(2B)-N(2)-Co(1)	105.9(6)

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

Complex 4:

Er(1)-O(6)#1	2.312(3)	Er(1)-O(6)	2.312(3)	Er(1)-O(3)#1	2.338(3)
Er(1)-O(3)	2.338(3)	Er(1)-O(2)	2.347(3)	Er(1)-O(2)#1	2.347(3)
Er(1)-O(7)	2.361(6)	Er(1)-O(1)#1	2.706(3)	Er(1)-O(1)	2.706(3)
Er(1)-Co(1)	3.2927(9)	Er(1)-Co(1)#1	3.2928(9)	Co(1)-O(2)	1.881(3)
Co(1)-N(1)	1.880(4)	Co(1)-O(3)	1.897(3)	Co(1)-N(2)	1.907(4)
Co(1)-O(4)	1.948(5)	Co(1)-O(5)	1.926(3)		

O(6)#1-Er(1)-O(6)	134.70(18)	O(6)#1-Er(1)-O(3)#1	75.35(12)
O(6)-Er(1)-O(3)#1	147.20(11)	O(6)#1-Er(1)-O(3)	147.21(11)
O(6)-Er(1)-O(3)	75.35(12)	O(3)#1-Er(1)-O(3)	80.56(14)
O(6)#1-Er(1)-O(2)	125.72(12)	O(6)-Er(1)-O(2)	74.35(11)
O(3)#1-Er(1)-O(2)	76.07(10)	O(3)-Er(1)-O(2)	67.58(9)
O(6)#1-Er(1)-O(2)#1	74.35(11)	O(6)-Er(1)-O(2)#1	125.72(12)
O(3)#1-Er(1)-O(2)#1	67.58(9)	O(3)-Er(1)-O(2)#1	76.07(10)
O(2)-Er(1)-O(2)#1	131.88(14)	O(6)#1-Er(1)-O(7)	67.35(9)
O(6)-Er(1)-O(7)	67.35(9)	O(3)#1-Er(1)-O(7)	139.72(7)
O(3)-Er(1)-O(7)	139.72(7)	O(2)-Er(1)-O(7)	114.06(7)
O(2)#1-Er(1)-O(7)	114.06(7)	O(6)#1-Er(1)-O(1)#1	94.36(12)
O(6)-Er(1)-O(1)#1	71.73(11)	O(3)#1-Er(1)-O(1)#1	126.88(9)
O(3)-Er(1)-O(1)#1	82.54(11)	O(2)-Er(1)-O(1)#1	139.33(10)
O(2)#1-Er(1)-O(1)#1	59.53(9)	O(7)-Er(1)-O(1)#1	72.04(8)
O(6)#1-Er(1)-O(1)	71.74(11)	O(6)-Er(1)-O(1)	94.35(12)
O(3)#1-Er(1)-O(1)	82.55(11)	O(3)-Er(1)-O(1)	126.88(9)
O(2)-Er(1)-O(1)	59.53(9)	O(2)#1-Er(1)-O(1)	139.33(10)
O(7)-Er(1)-O(1)	72.04(8)	O(1)#1-Er(1)-O(1)	144.09(15)
O(6)#1-Er(1)-Co(1)	153.68(10)	O(6)-Er(1)-Co(1)	66.18(9)
O(3)#1-Er(1)-Co(1)	81.36(7)	O(3)-Er(1)-Co(1)	34.36(6)
O(2)-Er(1)-Co(1)	34.00(6)	O(2)#1-Er(1)-Co(1)	107.92(8)
O(7)-Er(1)-Co(1)	129.747(17)	O(1)#1-Er(1)-Co(1)	109.53(8)
O(1)-Er(1)-Co(1)	93.43(7)	O(6)#1-Er(1)-Co(1)#1	66.18(9)
O(6)-Er(1)-Co(1)#1	153.68(10)	O(3)#1-Er(1)-Co(1)#1	34.37(6)
O(3)-Er(1)-Co(1)#1	81.37(7)	O(2)-Er(1)-Co(1)#1	107.92(8)

O(2)#1-Er(1)-Co(1)#1	34.00(6)	O(7)-Er(1)-Co(1)#1	129.747(17)
O(1)#1-Er(1)-Co(1)#1	93.43(7)	O(1)-Er(1)-Co(1)#1	109.53(8)
Co(1)-Er(1)-Co(1)#1	100.51(3)	O(2)-Co(1)-N(1)	97.09(14)
O(2)-Co(1)-O(3)	87.22(11)	N(1)-Co(1)-O(3)	175.69(14)
O(2)-Co(1)-N(2)	175.54(16)	N(1)-Co(1)-N(2)	87.30(17)
O(3)-Co(1)-N(2)	88.39(15)	O(2)-Co(1)-O(4)	87.39(17)
N(1)-Co(1)-O(4)	90.79(19)	O(3)-Co(1)-O(4)	89.31(17)
N(2)-Co(1)-O(4)	93.4(2)	O(2)-Co(1)-O(5)	92.35(14)
N(1)-Co(1)-O(5)	86.81(16)	O(3)-Co(1)-O(5)	93.12(13)
N(2)-Co(1)-O(5)	87.08(18)	O(4)-Co(1)-O(5)	177.54(18)
O(2)-Co(1)-Er(1)	44.25(8)	N(1)-Co(1)-Er(1)	140.15(12)
O(3)-Co(1)-Er(1)	44.09(8)	N(2)-Co(1)-Er(1)	131.29(14)
O(4)-Co(1)-Er(1)	95.54(13)	O(5)-Co(1)-Er(1)	85.96(10)
C(7)-O(2)-Co(1)	123.5(2)	C(7)-O(2)-Er(1)	131.1(3)
Co(1)-O(2)-Er(1)	101.75(11)	C(12)-O(3)-Co(1)	109.2(3)
C(12)-O(3)-Er(1)	139.9(3)	Co(1)-O(3)-Er(1)	101.55(11)
C(13)-O(5)-Co(1)	125.6(3)	C(2)-O(1)-Er(1)	117.1(2)
C(1)-O(1)-Er(1)	126.5(3)	C(13)-O(6)-Er(1)	136.0(3)
C(8)-N(1)-Co(1)	125.0(3)	C(9)-N(1)-Co(1)	112.0(3)
C(2A)-N(2)-Co(1)	108.5(4)	C(1A)-N(2)-Co(1)	107.1(4)
C(1B)-N(2)-Co(1)	109.2(7)	C(2B)-N(2)-Co(1)	108.5(9)

Symmetry transformations used to generate equivalent atoms:

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