Electronic Supplementary Information (ESI)

Ferrocenyl-based Di- and Trinuclear Lanthanide Complexes: Solid State structures, (Spectro)Electrochemical and DFT Studies

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Table of Contents

1- IR spectra

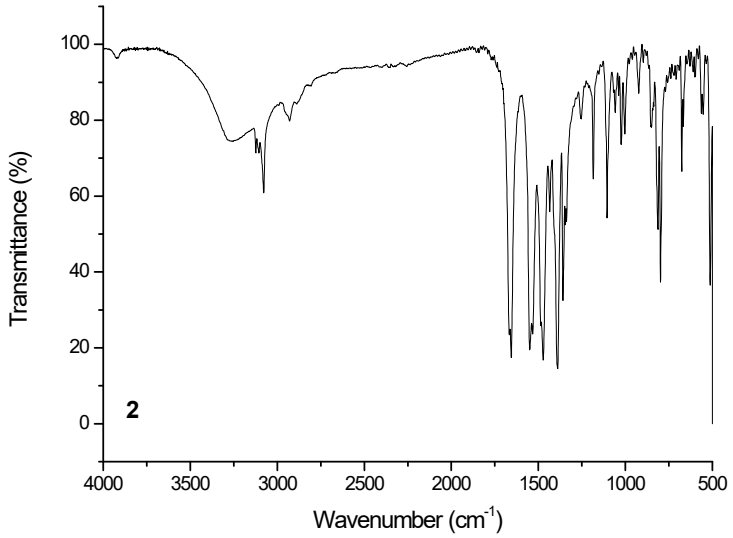


Figure S1. IR spectra of **2** (KBr).

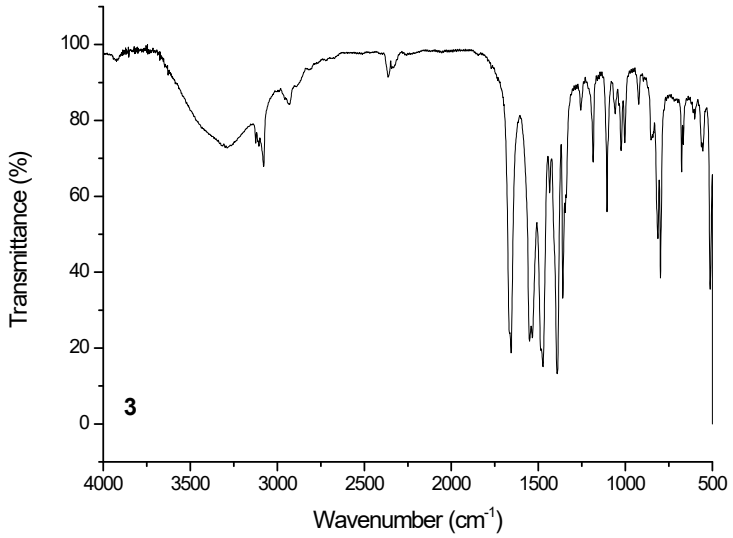


Figure S2. IR spectra of **3** (KBr).

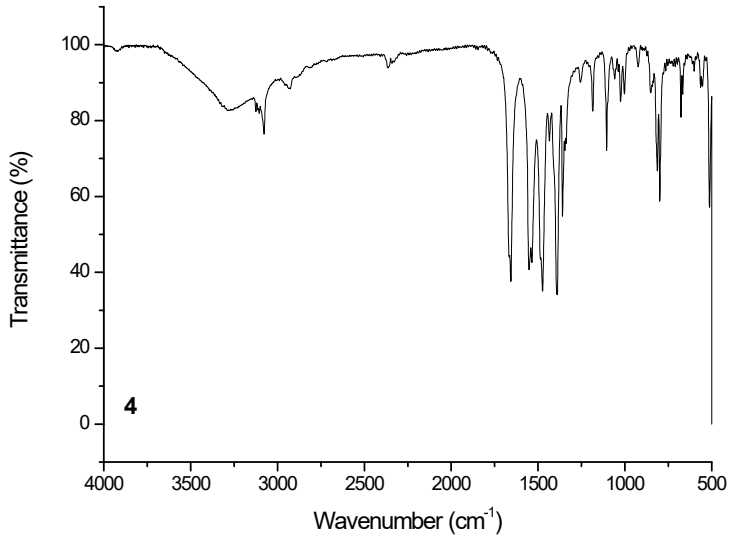


Figure S3. IR spectra of **4** (KBr).

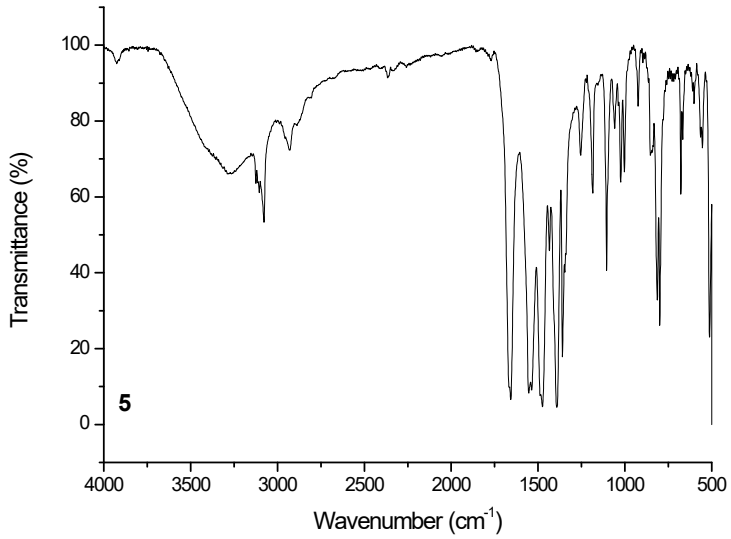


Figure S4. IR spectra of **5** (KBr).

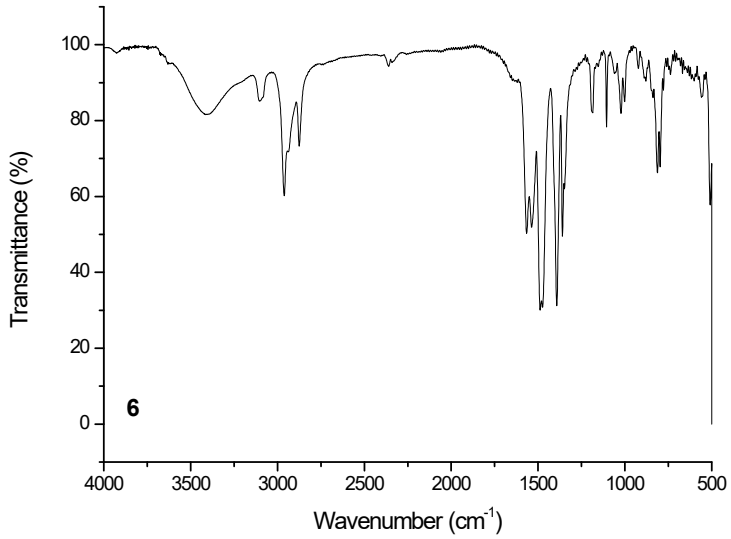


Figure S5. IR spectra of **6** (KBr).

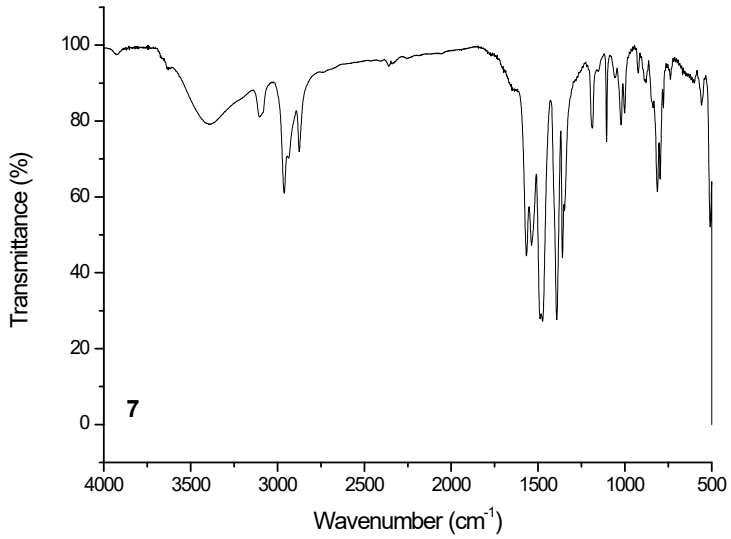


Figure S6. IR spectra of **7** (KBr).

2. Crystal data

Table S1. Comparison of the most likely coordination polyhedra in complexes **2** – **5** obtained via the SHAPE program package.[1]

Compound	M	JCSAPR[1)]	CSAPR[2)]	JTCTPR[3)]	TCTPR[4)]	Δ[3)–4)]	MFF[5)]
2	Sm	3.151	2.801	2.683	2.542	141	2.774
3	Eu	3.094	2.765	2.576	2.529	47	2.813
4	Gd	3.08	2.813	2.525	2.568	–43	2.853
5	Tb	2.937	2.824	2.423	2.553	–130	2.883

1) JCSAPR = Capped square antiprism; 2) CSAPR = Spherical capped square antiprism; 3) JTCTPR = Tricapped trigonal prism; 4) TCTPR = Spherical tricapped trigonal prism; 5) MFF = Muffin.

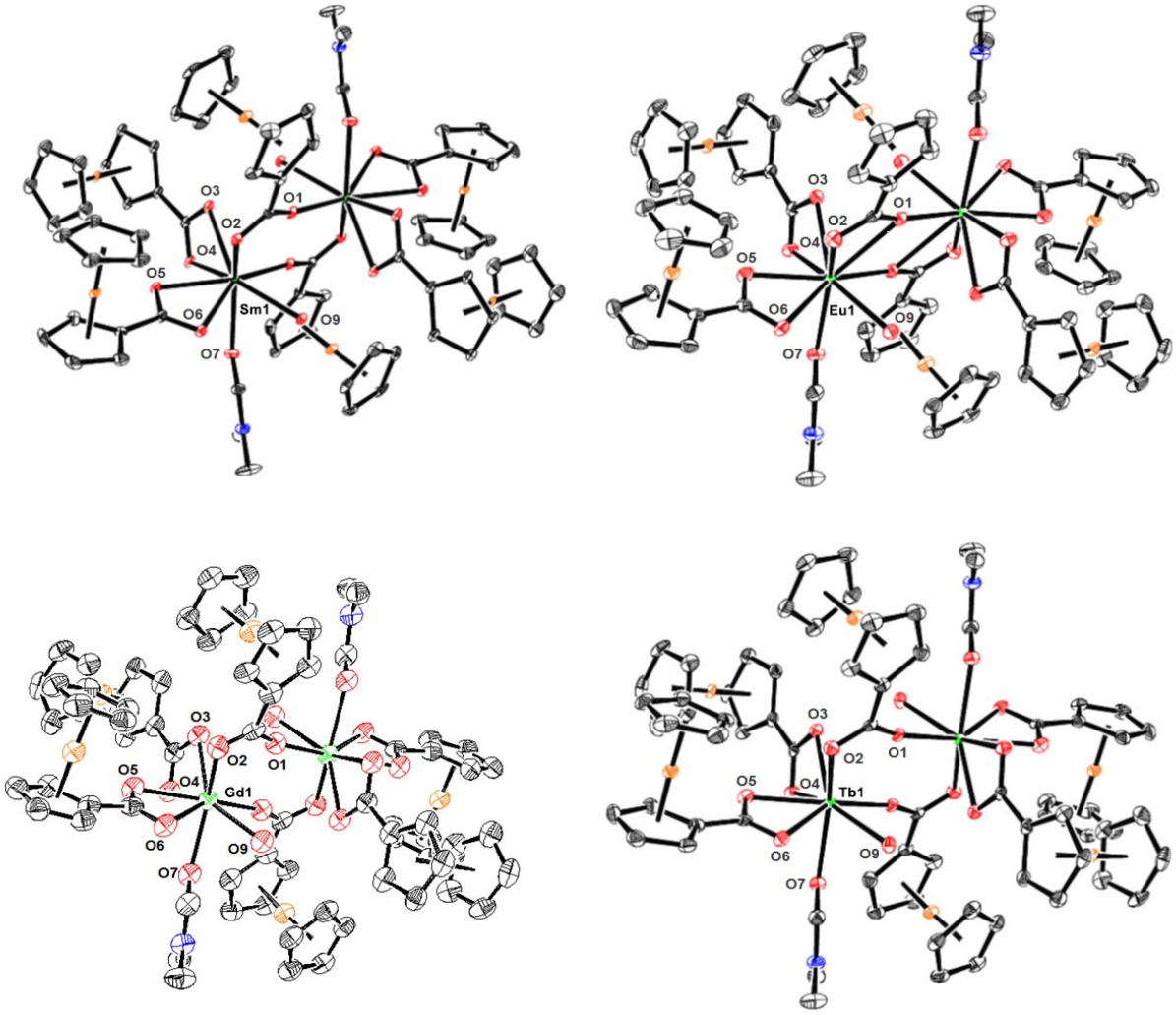


Figure S7. ORTEP diagram (50 % probability level) of the molecular structures of **2** (top, left), **3** (top, right), **4** (bottom, left) and **5** (bottom, right) with the atom-numbering scheme. All hydrogen atoms have been omitted for clarity. Symmetry operation for generating equivalent atoms: 1–x,1–y,–z.

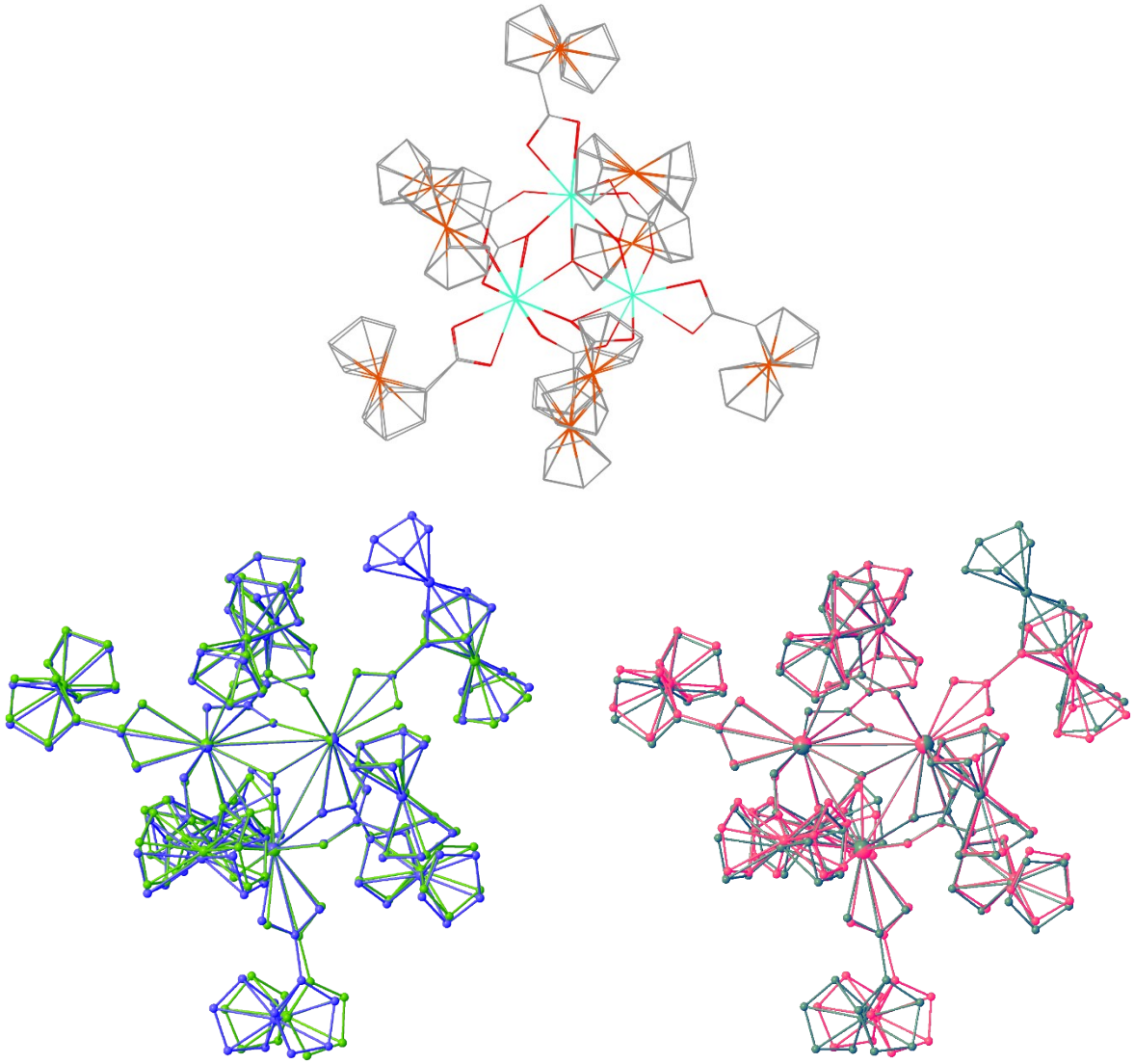


Figure S8. Top: Overlay of compounds **6** and **7** based on their Ln, Fe and μ^3-O atoms: RMSD: 0.0679 (0.012 Å if only Ln atoms are considered). Bottom: Overlay molecules 1 & 2 in **6** (Left; RMSD: 0.028 Å, based on Gd); in **7** (Right: RMSD: 0.026 Å)

Table S2. Comparison of the most likely coordination polyhedra in complexes **6** and **7** obtained via the SHAPE program.[1]

Compound	Atom	SAPR	TDD	BTPR	JGBF	JETBPY*	JBTPR	JSD
6	Gd1	27.098,	26.339,	26.898,	27.200,	17.632,	23.308,	23.664,
	Gd2	24.283,	24.900,	23.324,	27.128,	17.578,	20.694,	18.623,
	Gd3	20.239,	21.117,	20.076,	24.155,	18.988,	17.175,	17.160,
	Gd4	24.924,	25.617,	23.683,	25.996,	17.404,	20.682,	19.301,
	Gd5	20.748,	21.236,	20.433,	24.265,	19.466,	17.442,	17.077,
	Gd6	27.013,	26.673,	27.320,	26.679,	18.548,	24.139,	24.385,
7	TB1	20.251,	21.128,	20.112,	23.952,	18.558,	17.265,	17.330,
	Tb2	27.226,	26.408,	26.932,	27.003,	17.642,	23.465,	23.697,
	Tb3	24.459,	25.070,	23.633,	27.468,	17.773,	21.058,	18.888,
	Tb11	24.899,	25.648,	23.859,	26.328,	17.500,	21.030,	19.444,
	Tb12	20.342,	20.933,	20.113,	24.161,	19.556,	17.121,	16.846,
	Tb13	26.782,	26.426,	27.186,	26.542,	18.595,	23.974,	24.208,

SAPR = Square antiprism, TDD-8 = triangular dodecahedron, JETBPY* = Johnson elongated triangular bipyramid J14, JBTPR = Biaugmented trigonal prism J50, BTPR = Biaugmented trigonal prism, JSD = Snub diphenoid J84. * Could not be detected within the coordination spheres, thus the next closest regular shape was chosen.

Table S3. Orientation analysis of individual polyhedron orientations of **7** via the SHAPE program.[1]

Center	Orientation	prism	pyramid	average	average all	capps
TB1	**Tb1/2**	17.957	23.518/25.3	24.409	**21.183**	O1, O3
	Tb3	22.849	30.48/26.923	28.7015	25.77525	O2, O8
TB2	**Tb1/2**	26.805	27.133/30.933	29.033	**27.919**	O1, O5
	Tb3	26.782	31.501/31.579	31.54	29.161	O4, O8
TB3	Tb1/2	25.772	31.042/30.757	30.8995	28.33575	O1, O7
	Tb3	21.872	28.417/31.871	30.144	**26.008**	O15, O16

Table S4. The shortest distances between individual ferrocenyl groups in **7**, based on their Fe···Fe and ipso carbon C···C distances.

Fc[a)]	pattern	M[b)]	Fe···Fe	Fc'	pattern	M'
1	κ^2	1	6.7501(3)	6	$\mu\kappa^3$	2,1
7	κ^2	2	6.2146(2)	2	$\mu\kappa^3$	3,2
5	κ^2	3	6.5990(3)	8	$\mu\kappa^3$	1,3
3	$\mu\kappa^2$	2,1	6.4910(3)	4	$\mu\kappa^2$	3,2
9	$\mu\kappa^2$	3,1	6.7446(2)	3	$\mu\kappa^2$	2,1
4	$\mu\kappa^2$	3,2	6.4910(3)	3	$\mu\kappa^2$	2,1
8	$\mu\kappa^3$	1,3	6.5990(3)	5	κ^2	3
6	$\mu\kappa^3$	2,1	6.7501(3)	1	κ^2	1
2	$\mu\kappa^3$	3,2	6.2146(2)	7	κ^2	2

Fc[a)]	pattern	M[b)]	C···C	Fc'	pattern	M'
1	κ^2	1	5.5221(2)	6	$\mu\kappa^3$	2,1
7	κ^2	2	5.7192(2)	2	$\mu\kappa^3$	3,2
5	κ^2	3	5.8202(2)	9	$\mu\kappa^2$	3,1
3	$\mu\kappa^2$	2,1	6.3893(2)	1	κ^2	1
9	$\mu\kappa^2$	3,1	5.8202(2)	5	κ^2	3
4	$\mu\kappa^2$	3,2	6.0406(2)	2	$\mu\kappa^3$	3,2
8	$\mu\kappa^3$	1,3	5.4155(2)	6	$\mu\kappa^3$	2,1
6	$\mu\kappa^3$	2,1	5.4155(2)	8	$\mu\kappa^3$	1,3
2	$\mu\kappa^3$	3,2	5.7054(2)	6	$\mu\kappa^3$	2,1

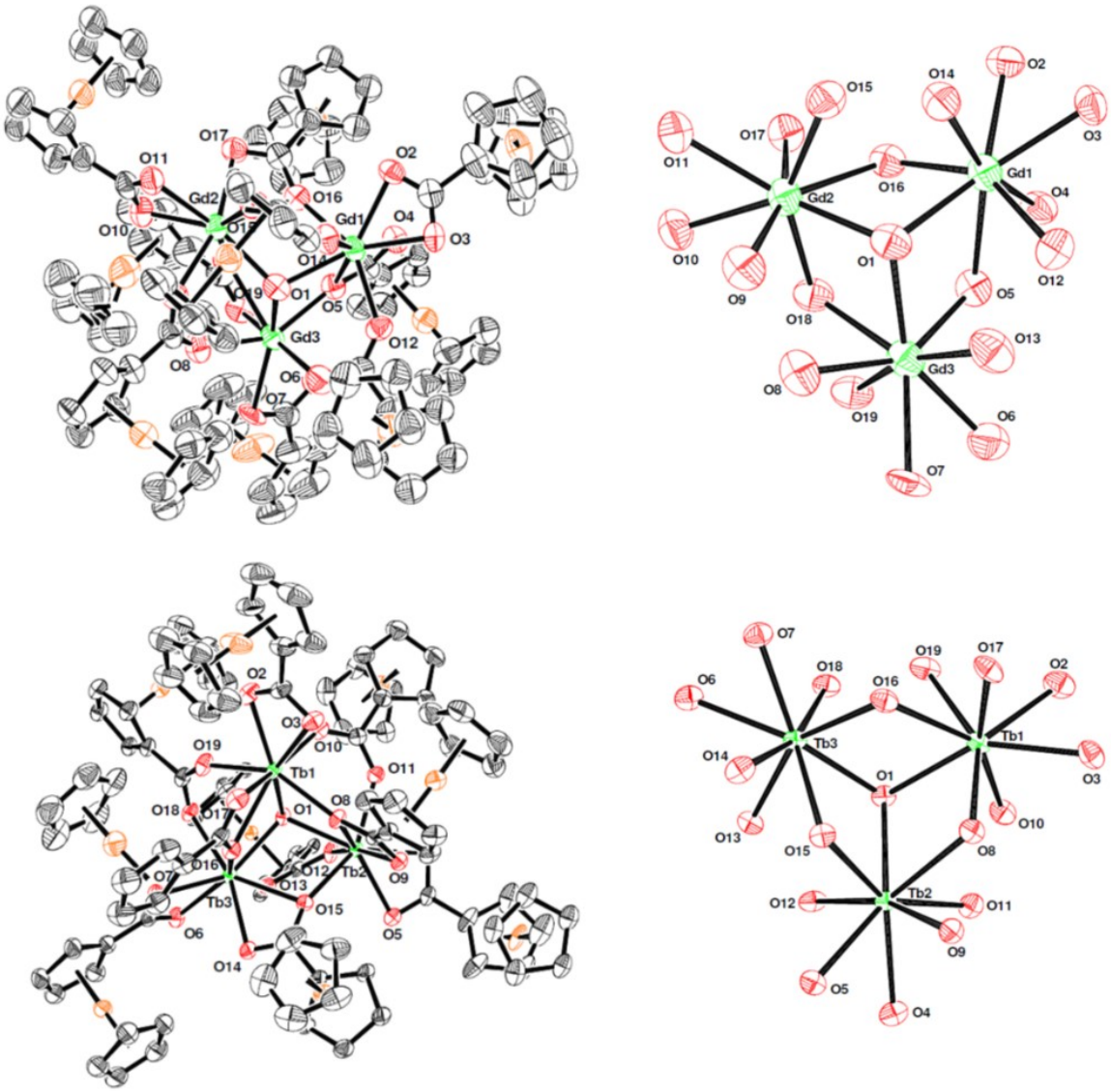


Figure S9. ORTEP diagram (50% probability level) of the molecular structures of **6** (top) and **7** (bottom) with the atom numbering scheme. All hydrogen atoms have been omitted for clarity.

Table S4A. Short Fe···Fe and ^{i}C···^{i}C distances for both molecules in the symmetric unit of **7** and the reference labeling in DFT structure **Y**.

Fc (DFT)	Fc (X-Ray)	mode	Fc (X-Ray)	mode	Fe···Fe / Å		^{i}C···^{i}C / Å	
					M 1	M 2	M 1	M 2
5	1	κ^2	1	κ^2				
			2	κ^2	12.9154(8)	12.749(3)	8.5711(6)	8.583(11)
			3	κ^2	12.3945(5)	12.791(3)	8.5602(4)	8.615(11)
			4	$\mu\kappa^3$	6.7173(3)	6.403(2)	5.0183(3)	4.978(10)
			5	$\mu\kappa^2$	9.3715(4)	9.563(3)	4.2335(2)	4.299(11)
			6	$\mu\kappa^2$	12.2757(6)	12.574(2)	8.0494(5)	8.111(11)
			7	$\mu\kappa^3$	10.2367(6)	9.890(3)	7.6630(4)	7.609(10)
			8	$\mu\kappa^3$	6.6844(3)	6.944(3)	4.5254(2)	4.469(11)
			9	$\mu\kappa^2$	7.7630(4)	8.314(3)	5.1861(2)	5.240(10)
1	2	κ^2	1	κ^2	12.9154(8)	12.749(3)	8.5711(6)	8.583(11)
			2	κ^2				
			3	κ^2	12.4977(6)	12.2784(18)	8.4565(4)	8.304(10)
			4	$\mu\kappa^3$	6.9014(5)	6.9597(18)	4.3895(3)	4.365(10)
			5	$\mu\kappa^2$	9.0753(4)	9.1734(18)	5.3218(3)	5.366(11)
			6	$\mu\kappa^2$	10.2366(6)	10.1913(16)	4.4434(2)	4.317(10)
			7	$\mu\kappa^3$	6.8045(4)	6.7193(19)	4.7889(3)	4.783(10)
			8	$\mu\kappa^3$	12.5879(5)	12.522(2)	7.6843(4)	7.687(11)
			9	$\mu\kappa^2$	13.2092(6)	13.2409(17)	8.2457(4)	8.228(10)
7	3	κ^2	1	κ^2	12.3945(5)	12.791(3)	8.5602(4)	8.615(11)
			2	κ^2	12.4977(6)	12.2784(18)	8.4565(4)	8.304(10)
			3	κ^2				
			4	$\mu\kappa^3$	12.4269(6)	12.6055(18)	7.6941(4)	7.687(10)
			5	$\mu\kappa^2$	13.2146(8)	12.995(2)	8.2861(5)	8.201(11)
			6	$\mu\kappa^2$	8.8524(5)	8.2648(19)	5.2754(3)	5.189(11)
			7	$\mu\kappa^3$	7.2242(4)	7.5043(16)	4.4670(2)	4.455(10)
			8	$\mu\kappa^3$	6.1575(3)	6.443(2)	4.9358(2)	5.020(10)
			9	$\mu\kappa^2$	9.9393(5)	9.8524(18)	4.3511(2)	4.352(11)
8	4	$\mu\kappa^3$	1	κ^2	6.7173(3)	6.403(2)	5.0183(3)	4.978(10)
			2	κ^2	6.9014(5)	6.9597(18)	4.3895(3)	4.365(10)
			3	κ^2	12.4269(6)	12.6055(18)	7.6941(4)	7.687(10)
			4	$\mu\kappa^3$				
			5	$\mu\kappa^2$	7.8918(4)	7.9695(16)	4.0836(2)	4.085(10)
			6	$\mu\kappa^2$	11.3672(7)	11.4352(15)	5.9790(3)	5.919(10)
			7	$\mu\kappa^3$	6.8305(3)	6.6944(18)	4.2820(2)	4.251(10)
			8	$\mu\kappa^3$	9.1256(4)	9.2504(19)	4.4381(2)	4.486(10)
			9	$\mu\kappa^2$	10.4946(6)	10.6047(17)	6.5669(4)	6.559(9)
9	5	$\mu\kappa^2$	1	κ^2	9.3715(4)	9.563(3)	4.2335(2)	4.299(11)
			2	κ^2	9.0753(4)	9.1734(18)	5.3218(3)	5.366(11)
			3	κ^2	13.2146(8)	12.995(2)	8.2861(5)	8.201(11)
			4	$\mu\kappa^3$	7.8918(4)	7.9695(16)	4.0836(2)	4.085(10)
			5	$\mu\kappa^2$				
			6	$\mu\kappa^2$	6.7516(3)	6.8320(17)	5.1796(2)	5.144(11)
			7	$\mu\kappa^3$	11.0573(5)	11.0140(18)	6.5066(3)	6.521(10)
			8	$\mu\kappa^3$	11.2365(7)	11.300(2)	6.0139(4)	6.003(11)
			9	$\mu\kappa^2$	6.8519(3)	6.8127(18)	5.3690(3)	5.328(10)
4	6	$\mu\kappa^2$	1	κ^2	12.2757(6)	12.574(2)	8.0494(5)	8.111(11)
			2	κ^2	10.2366(6)	10.1913(16)	4.4434(2)	4.317(10)
			3	κ^2	8.8524(5)	8.2648(19)	5.2754(3)	5.189(11)
			4	$\mu\kappa^3$	11.3672(7)	11.4352(15)	5.9790(3)	5.919(10)
			5	$\mu\kappa^2$	6.7516(3)	6.8320(17)	5.1796(2)	5.144(11)
			6	$\mu\kappa^2$				
			7	$\mu\kappa^3$	10.1277(6)	10.1012(16)	4.3097(2)	4.376(11)
			8	$\mu\kappa^3$	10.0518(4)	10.1021(18)	6.5601(3)	6.594(11)
			9	$\mu\kappa^2$	6.4412(4)	6.4693(14)	5.1433(3)	5.226(11)
6	7	$\mu\kappa^3$	1	κ^2	10.2367(6)	9.890(3)	7.6630(4)	7.609(10)
			2	κ^2	6.8045(4)	6.7193(19)	4.7889(3)	4.783(10)
			3	κ^2	7.2242(4)	7.5043(16)	4.4670(2)	4.455(10)
			4	$\mu\kappa^3$	6.8305(3)	6.6944(18)	4.2820(2)	4.251(10)
			5	$\mu\kappa^2$	11.0573(5)	11.0140(18)	6.5066(3)	6.521(10)
			6	$\mu\kappa^2$	10.1277(6)	10.1012(16)	4.3097(2)	4.376(11)
			7	$\mu\kappa^3$				
			8	$\mu\kappa^3$	7.2393(4)	7.1040(19)	4.3509(3)	4.326(10)
			9	$\mu\kappa^2$	11.3362(5)	11.3431(17)	5.9551(3)	5.967(10)

2	8	$\mu\kappa^3$	1	κ^2	6.6844(3)	6.944(3)	4.5254(2)	4.469(11)
			2	κ^2	12.5879(5)	12.522(2)	7.6843(4)	7.687(11)
			3	κ^2	6.1575(3)	6.443(2)	4.9358(2)	5.020(10)
			4	$\mu\kappa^3$	9.1256(4)	9.2504(19)	4.4381(2)	4.486(10)
			5	$\mu\kappa^2$	11.2365(7)	11.300(2)	6.0139(4)	6.003(11)
			6	$\mu\kappa^2$	10.0518(4)	10.1021(18)	6.5601(3)	6.594(11)
			7	$\mu\kappa^3$	7.2393(4)	7.1040(19)	4.3509(3)	4.326(10)
			8	$\mu\kappa^3$				
			9	$\mu\kappa^2$	7.3231(3)	7.4869(18)	4.1072(2)	4.067(9)
4	9	$\mu\kappa^2$	1	κ^2	7.7630(4)	8.314(3)	5.1861(2)	5.240(10)
			2	κ^2	13.2092(6)	13.2409(17)	8.2457(4)	8.228(10)
			3	κ^2	9.9393(5)	9.8524(18)	4.3511(2)	4.352(11)
			4	$\mu\kappa^3$	10.4946(6)	10.6047(17)	6.5669(4)	6.559(9)
			5	$\mu\kappa^2$	6.8519(3)	6.8127(18)	5.3690(3)	5.328(10)
			6	$\mu\kappa^2$	6.4412(4)	6.4693(14)	5.1433(3)	5.226(11)
			7	$\mu\kappa^3$	11.3362(5)	11.3431(17)	5.9551(3)	5.967(10)
			8	$\mu\kappa^3$	7.3231(3)	7.4869(18)	4.1072(2)	4.067(9)
			9	$\mu\kappa^2$				

Table S5. Bond lengths (Å) and angles (°) of complexes **2** - **5**.

2		**3**		**4**		**5**	
Bond lengths							
O(1)-Sm(1)	2.766(4)	O(1)-Eu(1)	2.779(2)	O(1)-Gd(1)	2.776(4)	O(1)-Tb(1)	2.819(2)
O(2)-Sm(1)	2.420(4)	O(2)-Eu(1)	2.405(2)	O(2)-Gd(1)	2.385(4)	O(2)-Tb(1)	2.373(2)
O(3)-Sm(1)	2.446(4)	O(3)-Eu(1)	2.433(2)	O(3)-Gd(1)	2.419(3)	O(3)-Tb(1)	2.4008(19)
O(4)-Sm(1)	2.557(4)	O(4)-Eu(1)	2.548(2)	O(4)-Gd(1)	2.541(3)	O(4)-Tb(1)	2.534(2)
O(5)-Sm(1)	2.419(4)	O(5)-Eu(1)	2.402(2)	O(5)-Gd(1)	2.383(4)	O(5)-Tb(1)	2.380(2)
O(6)-Sm(1)	2.521(4)	O(6)-Eu(1)	2.509(2)	O(6)-Gd(1)	2.503(3)	O(6)-Tb(1)	2.491(2)
O(7)-Sm(1)	2.432(4)	O(7)-Eu(1)	2.422(2)	O(7)-Gd(1)	2.400(4)	O(7)-Tb(1)	2.386(2)
O(9)-Sm(1)	2.462(4)	O(9)-Eu(1)	2.441(2)	O(9)-Gd(1)	2.422(3)	O(9)-Tb(1)	2.403(2)
O(1)^{i}-Sm(1)	2.379(4)	O(1)^{i}-Eu(1)	2.359(2)	O(1)^{i}-Gd(1)	2.349(4)	O(1)^{i}-Tb(1)	2.3178(19)
C(1)-O(1)	1.279(7)	C(1)-O(1)	1.282(4)	C(1)-O(1)	1.276(6)	C(1)-O(1)	1.278(3)
C(1)-O(2)	1.238(7)	C(1)-O(2)	1.256(5)	C(1)-O(2)	1.259(7)	C(1)-O(2)	1.255(4)
C(12)-O(3)	1.283(7)	C(12)-O(3)	1.289(4)	C(12)-O(3)	1.285(6)	C(12)-O(3)	1.284(4)
C(12)-O(4)	1.275(7)	C(12)-O(4)	1.256(4)	C(12)-O(4)	1.257(7)	C(12)-O(4)	1.251(4)
C(23)-O(5)	1.281(7)	C(23)-O(5)	1.287(4)	C(23)-O(5)	1.274(6)	C(23)-O(5)	1.273(3)
C(23)-O(6)	1.246(7)	C(23)-O(6)	1.259(4)	C(23)-O(6)	1.253(6)	C(23)-O(6)	1.256(4)
C(34)-O(7)	1.243(8)	C(34)-O(7)	1.246(5)	C(34)-O(7)	1.253(7)	C(34)-O(7)	1.253(4)
C(37)-O(8)	1.221(9)	C(37)-O(8)	1.223(6)	C(37)-O(8)	1.236(9)	C(37)-O(8)	1.226(5)
Bond angles							
O(1)^{i}-Sm(1)-O(5)	149.22(14)	O(1)^{i}-Eu(1)-O(5)	148.81(8)	O(1)^{i}-Gd(1)-O(5)	149.08(12)	O(1)^{i}-Tb(1)-O(5)	149.18(7)
O(1)^{i}-Sm(1)-O(2)	119.01(14)	O(1)^{i}-Eu(1)-O(2)	119.03(8)	O(1)^{i}-Gd(1)-O(2)	118.77(13)	O(1)^{i}-Tb(1)-O(2)	118.36(7)
O(5)-Sm(1)-O(2)	82.64(14)	O(5)-Eu(1)-O(2)	83.16(8)	O(5)-Gd(1)-O(2)	83.11(13)	O(5)-Tb(1)-O(2)	83.35(7)
O(1)^{i}-Sm(1)-O(7)	87.32(14)	O(1)^{i}-Eu(1)-O(7)	87.09(9)	O(1)^{i}-Gd(1)-O(7)	87.15(13)	O(1)^{i}-Tb(1)-O(7)	86.57(7)
O(5)-Sm(1)-O(7)	87.48(14)	O(5)-Eu(1)-O(7)	87.19(9)	O(5)-Gd(1)-O(7)	87.17(13)	O(5)-Tb(1)-O(7)	87.78(7)
O(2)-Sm(1)-O(7)	140.69(14)	O(2)-Eu(1)-O(7)	140.97(8)	O(2)-Gd(1)-O(7)	141.29(12)	O(2)-Tb(1)-O(7)	141.94(7)
O(1)^{i}-Sm(1)-O(3)	81.59(13)	O(1)^{i}-Eu(1)-O(3)	81.52(8)	O(1)^{i}-Gd(1)-O(3)	81.40(12)	O(1)^{i}-Tb(1)-O(3)	81.68(7)
O(5)-Sm(1)-O(3)	80.94(13)	O(5)-Eu(1)-O(3)	81.12(8)	O(5)-Gd(1)-O(3)	81.37(12)	O(5)-Tb(1)-O(3)	81.26(7)
O(2)-Sm(1)-O(3)	80.51(13)	O(2)-Eu(1)-O(3)	80.42(8)	O(2)-Gd(1)-O(3)	80.20(12)	O(2)-Tb(1)-O(3)	79.65(7)
O(7)-Sm(1)-O(3)	135.25(14)	O(7)-Eu(1)-O(3)	135.16(8)	O(7)-Gd(1)-O(3)	135.11(12)	O(7)-Tb(1)-O(3)	135.36(7)
O(1)^{i}-Sm(1)-O(9)	77.27(14)	O(1)^{i}-Eu(1)-O(9)	77.02(8)	O(1)^{i}-Gd(1)-O(9)	76.94(12)	O(1)^{i}-Tb(1)-O(9)	76.85(7)
O(5)-Sm(1)-O(9)	129.92(14)	O(5)-Eu(1)-O(9)	130.38(8)	O(5)-Gd(1)-O(9)	130.31(12)	O(5)-Tb(1)-O(9)	130.47(7)
O(2)-Sm(1)-O(9)	83.33(14)	O(2)-Eu(1)-O(9)	83.27(8)	O(2)-Gd(1)-O(9)	83.21(13)	O(2)-Tb(1)-O(9)	82.78(7)
O(7)-Sm(1)-O(9)	74.25(14)	O(7)-Eu(1)-O(9)	74.61(9)	O(7)-Gd(1)-O(9)	74.92(13)	O(7)-Tb(1)-O(9)	75.21(7)
O(3)-Sm(1)-O(9)	142.66(14)	O(3)-Eu(1)-O(9)	142.17(8)	O(3)-Gd(1)-O(9)	141.84(13)	O(3)-Tb(1)-O(9)	141.31(7)
O(1)^{i}-Sm(1)-O(6)	150.94(13)	O(1)^{i}-Eu(1)-O(6)	150.71(8)	O(1)^{i}-Gd(1)-O(6)	150.64(12)	O(1)^{i}-Tb(1)-O(6)	150.20(7)

O(5)-Sm(1)-O(6)	52.86(13)	O(5)-Eu(1)-O(6)	53.34(8)	O(5)-Gd(1)-O(6)	53.23(11)	O(5)-Tb(1)-O(6)	53.69(6)
O(2)-Sm(1)-O(6)	71.05(14)	O(2)-Eu(1)-O(6)	70.99(8)	O(2)-Gd(1)-O(6)	71.25(13)	O(2)-Tb(1)-O(6)	71.55(7)
O(7)-Sm(1)-O(6)	72.70(14)	O(7)-Eu(1)-O(6)	72.94(8)	O(7)-Gd(1)-O(6)	72.95(12)	O(7)-Tb(1)-O(6)	73.41(7)
O(3)-Sm(1)-O(6)	127.44(13)	O(3)-Eu(1)-O(6)	127.73(8)	O(3)-Gd(1)-O(6)	127.91(11)	O(3)-Tb(1)-O(6)	128.04(6)
O(9)-Sm(1)-O(6)	77.11(14)	O(9)-Eu(1)-O(6)	77.12(8)	O(9)-Gd(1)-O(6)	77.14(12)	O(9)-Tb(1)-O(6)	76.82(7)
O(1)^{i}-Sm(1)-O(4)	77.70(13)	O(1)^{i}-Eu(1)-O(4)	77.53(8)	O(1)^{i}-Gd(1)-O(4)	77.47(11)	O(1)^{i}-Tb(1)-O(4)	77.59(7)
O(5)-Sm(1)-O(4)	71.56(13)	O(5)-Eu(1)-O(4)	71.33(8)	O(5)-Gd(1)-O(4)	71.66(11)	O(5)-Tb(1)-O(4)	71.64(7)
O(2)-Sm(1)-O(4)	128.53(13)	O(2)-Eu(1)-O(4)	128.58(8)	O(2)-Gd(1)-O(4)	128.68(12)	O(2)-Tb(1)-O(4)	128.58(7)
O(7)-Sm(1)-O(4)	82.84(14)	O(7)-Eu(1)-O(4)	82.64(8)	O(7)-Gd(1)-O(4)	82.33(12)	O(7)-Tb(1)-O(4)	82.30(7)
O(3)-Sm(1)-O(4)	52.48(14)	O(3)-Eu(1)-O(4)	52.58(8)	O(3)-Gd(1)-O(4)	52.85(12)	O(3)-Tb(1)-O(4)	53.14(7)
O(9)-Sm(1)-O(4)	146.59(13)	O(9)-Eu(1)-O(4)	146.46(8)	O(9)-Gd(1)-O(4)	146.34(12)	O(9)-Tb(1)-O(4)	146.69(7)
O(6)-Sm(1)-O(4)	119.02(13)	O(6)-Eu(1)-O(4)	119.44(8)	O(6)-Gd(1)-O(4)	119.52(12)	O(6)-Tb(1)-O(4)	119.90(7)
O(1)^{i}-Sm(1)-O(1)	69.56(15)	O(1)^{i}-Eu(1)-O(1)	69.34(9)	O(1)^{i}-Gd(1)-O(1)	69.05(14)	O(1)^{i}-Tb(1)-O(1)	69.11(7)
O(5)-Sm(1)-O(1)	126.24(13)	O(5)-Eu(1)-O(1)	126.95(8)	O(5)-Gd(1)-O(1)	127.03(12)	O(5)-Tb(1)-O(1)	126.81(6)
O(2)-Sm(1)-O(1)	49.52(13)	O(2)-Eu(1)-O(1)	49.76(8)	O(2)-Gd(1)-O(1)	49.78(12)	O(2)-Tb(1)-O(1)	49.32(6)
O(7)-Sm(1)-O(1)	144.16(13)	O(7)-Eu(1)-O(1)	143.94(8)	O(7)-Gd(1)-O(1)	143.93(12)	O(7)-Tb(1)-O(1)	143.63(6)
O(3)-Sm(1)-O(1)	69.72(13)	O(3)-Eu(1)-O(1)	69.63(7)	O(3)-Gd(1)-O(1)	69.46(11)	O(3)-Tb(1)-O(1)	69.15(6)
O(9)-Sm(1)-O(1)	74.16(13)	O(9)-Eu(1)-O(1)	73.74(8)	O(9)-Gd(1)-O(1)	73.55(12)	O(9)-Tb(1)-O(1)	73.22(7)
O(6)-Sm(1)-O(1)	115.64(12)	O(6)-Eu(1)-O(1)	115.65(8)	O(6)-Gd(1)-O(1)	115.84(11)	O(6)-Tb(1)-O(1)	115.58(6)
O(4)-Sm(1)-O(1)	116.53(13)	O(4)-Eu(1)-O(1)	116.39(7)	O(4)-Gd(1)-O(1)	116.36(11)	O(4)-Tb(1)-O(1)	116.30(6)
C(1)-O(1)-Sm(1)	85.8(4)	C(1)-O(1)-Eu(1)	85.5(2)	C(1)-O(1)-Gd(1)	85.4(3)	C(1)-O(1)-Tb(1)	83.98(17)
C(1)-O(2)-Sm(1)	103.3(3)	C(1)-O(2)-Eu(1)	103.9(2)	C(1)-O(2)-Gd(1)	104.4(3)	C(1)-O(2)-Tb(1)	105.78(17)
C(12)-O(3)-Sm(1)	95.8(3)	C(12)-O(3)-Eu(1)	95.32(19)	C(12)-O(3)-Gd(1)	95.2(3)	C(12)-O(3)-Tb(1)	95.01(16)
C(12)-O(4)-Sm(1)	90.9(3)	C(12)-O(4)-Eu(1)	90.87(19)	C(12)-O(4)-Gd(1)	90.2(3)	C(12)-O(4)-Tb(1)	89.68(16)
C(23)-O(5)-Sm(1)	94.9(3)	C(23)-O(5)-Eu(1)	95.3(2)	C(23)-O(5)-Gd(1)	95.7(3)	C(23)-O(5)-Tb(1)	94.91(17)
C(23)-O(6)-Sm(1)	91.0(3)	C(23)-O(6)-Eu(1)	91.1(2)	C(23)-O(6)-Gd(1)	90.6(3)	C(23)-O(6)-Tb(1)	90.16(17)
C(34)-O(7)-Sm(1)	124.3(4)	C(34)-O(7)-Eu(1)	124.3(2)	C(34)-O(7)-Gd(1)	125.0(4)	C(34)-O(7)-Tb(1)	124.62(19)
O(2)-C(1)-O(1)	121.4(6)	O(2)-C(1)-O(1)	120.8(3)	O(2)-C(1)-O(1)	120.5(5)	O(2)-C(1)-O(1)	120.9(3)
O(4)-C(12)-O(3)	119.9(5)	O(4)-C(12)-O(3)	120.4(3)	O(4)-C(12)-O(3)	120.8(4)	O(4)-C(12)-O(3)	121.4(2)
O(6)-C(23)-O(5)	121.1(5)	O(6)-C(23)-O(5)	120.1(3)	O(6)-C(23)-O(5)	120.3(5)	O(6)-C(23)-O(5)	121.1(3)

Symmetry transformations used to generate equivalent atoms: i: -x,-y,-z+1

Table S6. Bond lengths (Å) and angles (°) of complexes **6** and **7**.

6		**7**	
Bond lengths			
O(1)-Gd(1)	2.404(10)	O(1)-Tb(1)	2.371(5)
O(2)-Gd(1)	2.412(8)	O(2)-Tb(1)	2.397(6)
O(3)-Gd(1)	2.391(9)	O(3)-Tb(1)	2.388(6)
O(4)-Gd(1)	2.438(10)	O(8)-Tb(1)	2.344(5)
O(5)-Gd(1)	2.573(11)	O(10)-Tb(1)	2.321(6)
O(12)-Gd(1)	2.335(10)	O(16)-Tb(1)	2.619(6)
O(14)-Gd(1)	2.356(10)	O(17)-Tb(1)	2.382(5)
O(16)-Gd(1)	2.350(11)	O(19)-Tb(1)	2.293(5)
O(1)-Gd(2)	2.386(11)	O(1)-Tb(2)	2.386(5)
O(9)-Gd(2)	2.358(10)	O(4)-Tb(2)	2.392(5)
O(10)-Gd(2)	2.365(11)	O(5)-Tb(2)	2.411(5)
O(11)-Gd(2)	2.431(12)	O(8)-Tb(2)	2.539(5)
O(15)-Gd(2)	2.310(11)	O(9)-Tb(2)	2.392(5)
O(16)-Gd(2)	2.531(10)	O(11)-Tb(2)	2.308(5)
O(17)-Gd(2)	2.441(10)	O(12)-Tb(2)	2.356(5)
O(18)-Gd(2)	2.390(10)	O(15)-Tb(2)	2.339(5)
O(1)-Gd(3)	2.383(9)	O(1)-Tb(3)	2.376(5)
O(5)-Gd(3)	2.330(10)	O(6)-Tb(3)	2.449(6)
O(6)-Gd(3)	2.411(12)	O(7)-Tb(3)	2.349(6)
O(7)-Gd(3)	2.416(9)	O(13)-Tb(3)	2.306(5)
O(8)-Gd(3)	2.304(11)	O(14)-Tb(3)	2.415(5)
O(13)-Gd(3)	2.350(12)	O(15)-Tb(3)	2.506(5)
O(18)-Gd(3)	2.622(12)	O(16)-Tb(3)	2.357(5)
O(19)-Gd(3)	2.407(11)	O(18)-Tb(3)	2.372(5)
O(21)-Gd(4)	2.358(11)	O(100)-Tb(11)	2.378(5)
O(22)-Gd(4)	2.401(10)	O(102)-Tb(11)	2.377(5)
O(23)-Gd(4)	2.410(11)	O(103)-Tb(11)	2.387(5)
O(24)-Gd(4)	2.427(10)	O(108)-Tb(11)	2.294(5)
O(25)-Gd(4)	2.525(10)	O(115)-Tb(11)	2.367(5)
O(32)-Gd(4)	2.324(12)	O(117)-Tb(11)	2.362(5)
O(34)-Gd(4)	2.356(10)	O(118)-Tb(11)	2.508(5)
O(36)-Gd(4)	2.379(11)	O(119)-Tb(11)	2.407(5)
O(21)-Gd(5)	2.385(9)	O(100)-Tb(12)	2.372(5)
O(29)-Gd(5)	2.352(11)	O(106)-Tb(12)	2.367(5)
O(30)-Gd(5)	2.383(11)	O(107)-Tb(12)	2.409(5)
O(31)-Gd(5)	2.384(8)	O(111)-Tb(12)	2.330(5)
O(35)-Gd(5)	2.330(10)	O(113)-Tb(12)	2.342(5)
O(36)-Gd(5)	2.553(11)	O(114)-Tb(12)	2.309(5)
O(37)-Gd(5)	2.405(11)	O(116)-Tb(12)	2.387(5)
O(38)-Gd(5)	2.333(10)	O(117)-Tb(12)	2.562(5)
O(21)-Gd(6)	2.398(9)	O(100)-Tb(13)	2.367(5)
O(25)-Gd(6)	2.336(10)	O(104)-Tb(13)	2.386(5)
O(26)-Gd(6)	2.404(7)	O(105)-Tb(13)	2.411(5)
O(27)-Gd(6)	2.396(10)	O(109)-Tb(13)	2.382(5)
O(28)-Gd(6)	2.336(10)	O(110)-Tb(13)	2.312(5)
O(33)-Gd(6)	2.426(11)	O(112)-Tb(13)	2.388(5)
O(38)-Gd(6)	2.587(11)	O(113)-Tb(13)	2.543(5)
O(39)-Gd(6)	2.425(10)	O(118)-Tb(13)	2.339(5)
C(1)-O(2)	1.26(2)	C(1)-O(2)	1.260(11)
C(1)-O(3)	1.22(2)	C(1)-O(3)	1.274(10)
C(12)-O(4)	1.303(16)	C(12)-O(4)	1.275(10)
C(12)-O(5)	1.273(17)	C(12)-O(5)	1.269(9)
C(23)-O(6)	1.289(18)	C(23)-O(6)	1.254(10)
C(23)-O(7)	1.30(2)	C(23)-O(7)	1.287(10)
C(34)-O(8)	1.28(2)	C(34)-O(8)	1.269(9)
C(34)-O(9)	1.26(2)	C(34)-O(9)	1.255(9)
C(45)-O(10)	1.30(2)	C(45)-O(10)	1.246(10)

C(45)-O(11)	1.229(19)	C(45)-O(11)	1.268(9)
C(56)-O(12)	1.284(17)	C(56)-O(12)	1.252(9)
C(56)-O(13)	1.275(18)	C(56)-O(13)	1.260(9)
C(67)-O(14)	1.252(19)	C(67)-O(14)	1.262(9)
C(67)-O(15)	1.24(2)	C(67)-O(15)	1.277(9)
C(78)-O(16)	1.32(2)	C(78)-O(16)	1.278(9)
C(78)-O(17)	1.288(19)	C(78)-O(17)	1.274(10)
C(89)-O(18)	1.232(18)	C(89)-O(18)	1.245(10)
C(89)-O(19)	1.29(2)	C(89)-O(19)	1.278(10)
C(101)-O(22)	1.25(2)	C(101)-O(102)	1.265(9)
C(101)-O(23)	1.33(2)	C(101)-O(103)	1.258(10)
C(112)-O(24)	1.288(19)	C(112)-O(104)	1.278(9)
C(112)-O(25)	1.258(18)	C(112)-O(105)	1.263(9)
C(123)-O(26)	1.242(19)	C(123)-O(106)	1.270(9)
C(123)-O(27)	1.285(18)	C(123)-O(107)	1.263(10)
C(134)-O(28)	1.235(17)	C(134)-O(108)	1.276(9)
C(134)-O(29)	1.276(19)	C(134)-O(109)	1.254(9)
C(145)-O(30)	1.278(18)	C(145)-O(110)	1.271(9)
C(145)-O(31)	1.27(2)	C(145)-O(111)	1.244(9)
C(156)-O(32)	1.24(2)	C(156)-O(112)	1.243(9)
C(156)-O(33)	1.276(19)	C(156)-O(113)	1.282(8)
C(167)-O(34)	1.266(18)	C(167)-O(114)	1.273(9)
C(167)-O(35)	1.259(19)	C(167)-O(115)	1.257(9)
C(178)-O(36)	1.27(2)	C(178)-O(116)	1.244(9)
C(178)-O(37)	1.27(2)	C(178)-O(117)	1.271(9)
C(189)-O(38)	1.262(17)	C(189)-O(118)	1.293(9)
C(189)-O(39)	1.270(18)	C(189)-O(119)	1.254(9)
Bond angles			
O(3)-Gd(1)-O(1)	150.4(4)	O(1)-Tb(1)-O(3)	145.23(18)
O(12)-Gd(1)-O(2)	132.9(4)	O(19)-Tb(1)-O(10)	102.1(2)
O(16)-Gd(1)-O(2)	79.8(4)	O(19)-Tb(1)-O(8)	146.3(2)
O(14)-Gd(1)-O(2)	82.3(4)	O(10)-Tb(1)-O(8)	88.40(19)
O(3)-Gd(1)-O(2)	53.8(4)	O(19)-Tb(1)-O(1)	78.65(18)
O(1)-Gd(1)-O(2)	141.0(4)	O(10)-Tb(1)-O(1)	74.43(18)
O(12)-Gd(1)-O(4)	93.0(4)	O(19)-Tb(1)-O(17)	90.2(2)
O(16)-Gd(1)-O(4)	85.9(4)	O(10)-Tb(1)-O(17)	161.6(2)
O(14)-Gd(1)-O(4)	163.0(3)	O(8)-Tb(1)-O(17)	88.77(19)
O(3)-Gd(1)-O(4)	81.3(4)	O(1)-Tb(1)-O(17)	121.99(18)
O(1)-Gd(1)-O(4)	121.5(3)	O(19)-Tb(1)-O(3)	130.9(2)
O(2)-Gd(1)-O(4)	81.1(4)	O(10)-Tb(1)-O(3)	80.7(2)
O(12)-Gd(1)-O(5)	76.4(4)	O(8)-Tb(1)-O(3)	82.10(18)
O(16)-Gd(1)-O(5)	76.5(3)	O(8)-Tb(1)-O(1)	73.45(17)
O(14)-Gd(1)-O(5)	143.6(3)	O(17)-Tb(1)-O(3)	80.9(2)
O(3)-Gd(1)-O(5)	125.9(4)	O(19)-Tb(1)-O(2)	76.7(2)
O(1)-Gd(1)-O(5)	69.1(3)	O(10)-Tb(1)-O(2)	81.2(2)
O(2)-Gd(1)-O(5)	129.2(4)	O(8)-Tb(1)-O(2)	137.0(2)
O(4)-Gd(1)-O(5)	53.1(3)	O(1)-Tb(1)-O(2)	140.52(18)
O(12)-Gd(1)-O(16)	146.8(4)	O(17)-Tb(1)-O(2)	88.5(2)
O(12)-Gd(1)-O(14)	95.3(4)	O(3)-Tb(1)-O(2)	55.1(2)
O(16)-Gd(1)-O(14)	95.1(4)	O(19)-Tb(1)-O(16)	73.08(19)
O(12)-Gd(1)-O(3)	79.1(4)	O(10)-Tb(1)-O(16)	144.42(18)
O(16)-Gd(1)-O(3)	133.2(4)	O(8)-Tb(1)-O(16)	79.77(18)
O(14)-Gd(1)-O(3)	85.7(4)	O(1)-Tb(1)-O(16)	70.05(16)
O(12)-Gd(1)-O(1)	81.0(4)	O(17)-Tb(1)-O(16)	52.38(18)
O(16)-Gd(1)-O(1)	71.6(3)	O(3)-Tb(1)-O(16)	129.75(18)
O(14)-Gd(1)-O(1)	74.6(3)	O(2)-Tb(1)-O(16)	129.18(19)
O(15)-Gd(2)-O(9)	97.8(4)	O(11)-Tb(2)-O(15)	146.44(19)
O(15)-Gd(2)-O(10	133.7(4)	O(11)-Tb(2)-O(12)	95.23(19)
O(9)-Gd(2)-O(10)	80.1(4)	O(15)-Tb(2)-O(12)	95.20(18)
O(15)-Gd(2)-O(18)	146.8(4)	O(11)-Tb(2)-O(1)	80.98(18)
O(9)-Gd(2)-O(18)	92.3(4)	O(15)-Tb(2)-O(1)	71.32(17)

O(10)-Gd(2)-O(18)	79.1(4)	O(12)-Tb(2)-O(1)	74.43(17)
O(15)-Gd(2)-O(1)	77.4(4)	O(11)-Tb(2)-O(4)	78.84(19)
O(9)-Gd(2)-O(1)	75.4(4)	O(15)-Tb(2)-O(4)	133.72(19)
O(10)-Gd(2)-O(1)	143.1(4)	O(12)-Tb(2)-O(4)	85.86(17)
O(1)-Gd(2)-O(18)	74.7(4)	O(1)-Tb(2)-O(4)	150.24(17)
O(15)-Gd(2)-O(11)	79.8(4)	O(11)-Tb(2)-O(9)	92.19(18)
O(9)-Gd(2)-O(11)	84.8(4)	O(15)-Tb(2)-O(9)	86.69(18)
O(10)-Gd(2)-O(11)	54.0(4)	O(12)-Tb(2)-O(9)	163.33(18)
O(18)-Gd(2)-O(11)	132.9(4)	O(1)-Tb(2)-O(9)	121.58(17)
O(1)-Gd(2)-O(11)	147.2(4)	O(4)-Tb(2)-O(9)	80.96(18)
O(15)-Gd(2)-O(17)	91.2(4)	O(11)-Tb(2)-O(5)	133.71(19)
O(9)-Gd(2)-O(17)	161.8(4)	O(15)-Tb(2)-O(5)	79.33(18)
O(10)-Gd(2)-O(17)	82.2(4)	O(12)-Tb(2)-O(5)	82.43(18)
O(18)-Gd(2)-O(17)	88.7(4)	O(1)-Tb(2)-O(5)	140.30(18)
O(1)-Gd(2)-O(17)	122.3(4)	O(4)-Tb(2)-O(5)	54.87(19)
O(11)-Gd(2)-O(17)	81.2(4)	O(9)-Tb(2)-O(5)	81.65(17)
O(15)-Gd(2)-O(16)	76.9(4)	O(11)-Tb(2)-O(8)	75.84(18)
O(9)-Gd(2)-O(16)	144.2(4)	O(15)-Tb(2)-O(8)	77.02(18)
O(10)-Gd(2)-O(16)	129.0(4)	O(12)-Tb(2)-O(8)	144.01(17)
O(18)-Gd(2)-O(16)	76.5(3)	O(1)-Tb(2)-O(8)	69.77(16)
O(1)-Gd(2)-O(16)	68.8(3)	O(4)-Tb(2)-O(8)	124.96(17)
O(11)-Gd(2)-O(16)	127.7(3)	O(9)-Tb(2)-O(8)	52.50(17)
O(17)-Gd(2)-O(16)	53.5(4)	O(5)-Tb(2)-O(8)	128.90(16)
O(8)-Gd(3)-O(5)	146.9(4)	O(13)-Tb(3)-O(7)	133.36(19)
O(8)-Gd(3)-O(13)	102.1(4)	O(13)-Tb(3)-O(16)	147.30(19)
O(5)-Gd(3)-O(13)	89.1(4)	O(7)-Tb(3)-O(16)	79.13(19)
O(8)-Gd(3)-O(1)	79.4(4)	O(13)-Tb(3)-O(18)	96.27(18)
O(5)-Gd(3)-O(1)	73.7(4)	O(7)-Tb(3)-O(18)	79.95(19)
O(13)-Gd(3)-O(1)	74.8(4)	O(16)-Tb(3)-O(18)	92.95(19)
O(8)-Gd(3)-O(6)	131.4(4)	O(13)-Tb(3)-O(1)	77.40(18)
O(5)-Gd(3)-O(6)	80.7(4)	O(7)-Tb(3)-O(1)	142.79(19)
O(13)-Gd(3)-O(6)	80.9(5)	O(16)-Tb(3)-O(1)	74.68(17)
O(1)-Gd(3)-O(6)	144.6(4)	O(18)-Tb(3)-O(1)	75.52(18)
O(8)-Gd(3)-O(19)	90.3(4)	O(13)-Tb(3)-O(14)	92.28(18)
O(5)-Gd(3)-O(19)	87.8(4)	O(7)-Tb(3)-O(14)	83.21(19)
O(13)-Gd(3)-O(19)	161.4(4)	O(16)-Tb(3)-O(14)	87.86(19)
O(1)-Gd(3)-O(19)	121.6(4)	O(18)-Tb(3)-O(14)	162.67(19)
O(19)-Gd(3)-O(6)	80.5(4)	O(1)-Tb(3)-O(14)	121.20(17)
O(8)-Gd(3)-O(7)	76.9(4)	O(13)-Tb(3)-O(6)	78.73(19)
O(5)-Gd(3)-O(7)	135.9(4)	O(7)-Tb(3)-O(6)	54.67(19)
O(13)-Gd(3)-O(7)	81.2(4)	O(16)-Tb(3)-O(6)	133.36(19)
O(1)-Gd(3)-O(7)	141.7(4)	O(18)-Tb(3)-O(6)	85.63(19)
O(6)-Gd(3)-O(7)	55.4(4)	O(1)-Tb(3)-O(6)	147.56(17)
O(19)-Gd(3)-O(7)	88.2(4)	O(14)-Tb(3)-O(6)	81.29(18)
O(8)-Gd(3)-O(18)	73.2(4)	O(13)-Tb(3)-O(15)	78.01(17)
O(5)-Gd(3)-O(18)	80.0(4)	O(7)-Tb(3)-O(15)	129.42(18)
O(13)-Gd(3)-O(18)	145.4(4)	O(16)-Tb(3)-O(15)	76.22(18)
O(1)-Gd(3)-O(18)	70.6(3)	O(18)-Tb(3)-O(15)	144.11(18)
O(6)-Gd(3)-O(18)	128.6(4)	O(1)-Tb(3)-O(15)	68.64(16)
O(19)-Gd(3)-O(18)	51.7(3)	O(14)-Tb(3)-O(15)	52.64(17)
O(7)-Gd(3)-O(18)	128.6(4)	O(6)-Tb(3)-O(15)	126.66(18)
O(32)-Gd(4)-O(34)	103.3(4)	O(108)-Tb(11)-O(117)	144.91(19)
O(32)-Gd(4)-O(21)	75.2(4)	O(108)-Tb(11)-O(115)	100.33(18)
O(34)-Gd(4)-O(21)	74.8(4)	O(117)-Tb(11)-O(115)	89.66(17)
O(32)-Gd(4)-O(36)	142.3(4)	O(108)-Tb(11)-O(102)	132.62(19)
O(34)-Gd(4)-O(36)	88.6(4)	O(117)-Tb(11)-O(102)	82.15(18)
O(21)-Gd(4)-O(36)	73.6(4)	O(115)-Tb(11)-O(102)	79.24(18)
O(32)-Gd(4)-O(22)	134.6(5)	O(108)-Tb(11)-O(100)	76.23(18)
O(34)-Gd(4)-O(22)	78.3(4)	O(117)-Tb(11)-O(100)	74.04(17)
O(21)-Gd(4)-O(22)	144.2(4)	O(115)-Tb(11)-O(100)	75.07(17)
O(36)-Gd(4)-O(22)	82.6(4)	O(102)-Tb(11)-O(100)	144.74(18)

O(32)-Gd(4)-O(23)	79.1(5)	O(108)-Tb(11)-O(103)	77.7(2)
O(34)-Gd(4)-O(23)	84.4(4)	O(117)-Tb(11)-O(103)	137.07(19)
O(21)-Gd(4)-O(23)	141.9(4)	O(115)-Tb(11)-O(103)	84.38(18)
O(36)-Gd(4)-O(23)	138.2(4)	O(102)-Tb(11)-O(103)	54.95(19)
O(22)-Gd(4)-O(23)	55.7(4)	O(100)-Tb(11)-O(103)	143.05(17)
O(32)-Gd(4)-O(24)	90.5(4)	O(108)-Tb(11)-O(119)	92.14(18)
O(34)-Gd(4)-O(24)	160.3(4)	O(117)-Tb(11)-O(119)	88.33(18)
O(21)-Gd(4)-O(24)	123.0(4)	O(115)-Tb(11)-O(119)	160.87(18)
O(36)-Gd(4)-O(24)	88.9(4)	O(102)-Tb(11)-O(119)	81.64(18)
O(22)-Gd(4)-O(24)	81.9(4)	O(100)-Tb(11)-O(119)	122.41(16)
O(23)-Gd(4)-O(24)	84.5(4)	O(103)-Tb(11)-O(119)	84.17(18)
O(32)-Gd(4)-O(25)	73.1(4)	O(108)-Tb(11)-O(118)	75.64(18)
O(34)-Gd(4)-O(25)	143.7(4)	O(117)-Tb(11)-O(118)	76.80(17)
O(21)-Gd(4)-O(25)	69.3(3)	O(115)-Tb(11)-O(118)	144.30(17)
O(36)-Gd(4)-O(25)	76.3(3)	O(102)-Tb(11)-O(118)	129.84(17)
O(22)-Gd(4)-O(25)	130.5(4)	O(100)-Tb(11)-O(118)	69.49(16)
O(23)-Gd(4)-O(25)	128.3(3)	O(103)-Tb(11)-O(118)	127.64(18)
O(24)-Gd(4)-O(25)	53.8(3)	O(119)-Tb(11)-O(118)	53.07(16)
O(35)-Gd(5)-O(38)	148.1(4)	O(114)-Tb(12)-O(111)	100.21(19)
O(35)-Gd(5)-O(29)	100.7(4)	O(114)-Tb(12)-O(113)	147.19(18)
O(38)-Gd(5)-O(29)	88.0(4)	O(111)-Tb(12)-O(113)	88.59(18)
O(35)-Gd(5)-O(30)	130.7(4)	O(114)-Tb(12)-O(106)	131.44(18)
O(38)-Gd(5)-O(30)	80.7(4)	O(111)-Tb(12)-O(106)	80.95(19)
O(29)-Gd(5)-O(30)	81.3(4)	O(113)-Tb(12)-O(106)	80.98(17)
O(35)-Gd(5)-O(31)	75.7(4)	O(114)-Tb(12)-O(100)	79.60(17)
O(38)-Gd(5)-O(31)	136.1(4)	O(111)-Tb(12)-O(100)	74.19(18)
O(29)-Gd(5)-O(31)	82.5(4)	O(113)-Tb(12)-O(100)	72.47(16)
O(31)-Gd(5)-O(30)	55.5(4)	O(106)-Tb(12)-O(100)	143.68(18)
O(35)-Gd(5)-O(21)	79.5(4)	O(114)-Tb(12)-O(116)	90.55(18)
O(38)-Gd(5)-O(21)	73.3(3)	O(111)-Tb(12)-O(116)	162.09(19)
O(29)-Gd(5)-O(21)	74.9(4)	O(113)-Tb(12)-O(116)	90.03(18)
O(30)-Gd(5)-O(21)	144.9(4)	O(106)-Tb(12)-O(116)	81.20(19)
O(31)-Gd(5)-O(21)	142.5(4)	O(100)-Tb(12)-O(116)	122.24(18)
O(35)-Gd(5)-O(37)	90.8(4)	O(114)-Tb(12)-O(107)	77.01(19)
O(38)-Gd(5)-O(37)	89.4(4)	O(111)-Tb(12)-O(107)	82.42(19)
O(29)-Gd(5)-O(37)	162.0(4)	O(113)-Tb(12)-O(107)	135.73(18)
O(30)-Gd(5)-O(37)	80.8(4)	O(106)-Tb(12)-O(107)	54.83(19)
O(31)-Gd(5)-O(37)	87.1(4)	O(100)-Tb(12)-O(107)	143.18(18)
O(21)-Gd(5)-O(37)	121.2(4)	O(116)-Tb(12)-O(107)	86.15(19)
O(35)-Gd(5)-O(36)	74.3(4)	O(114)-Tb(12)-O(117)	73.97(17)
O(38)-Gd(5)-O(36)	81.0(3)	O(111)-Tb(12)-O(117)	144.73(17)
O(29)-Gd(5)-O(36)	144.9(3)	O(113)-Tb(12)-O(117)	80.65(16)
O(30)-Gd(5)-O(36)	128.8(4)	O(106)-Tb(12)-O(117)	129.42(17)
O(31)-Gd(5)-O(36)	127.5(4)	O(100)-Tb(12)-O(117)	70.54(16)
O(21)-Gd(5)-O(36)	70.1(4)	O(116)-Tb(12)-O(117)	52.19(17)
O(37)-Gd(5)-O(36)	51.6(4)	O(107)-Tb(12)-O(117)	127.78(18)
O(28)-Gd(6)-O(25)	144.5(4)	O(110)-Tb(13)-O(118)	144.80(18)
O(25)-Gd(6)-O(27)	132.6(3)	O(110)-Tb(13)-O(100)	79.62(17)
O(28)-Gd(6)-O(27)	80.5(4)	O(118)-Tb(13)-O(100)	72.61(16)
O(25)-Gd(6)-O(21)	71.9(4)	O(110)-Tb(13)-O(109)	92.63(19)
O(28)-Gd(6)-O(21)	80.5(4)	O(118)-Tb(13)-O(109)	101.10(18)
O(27)-Gd(6)-O(21)	152.2(4)	O(100)-Tb(13)-O(109)	76.18(17)
O(25)-Gd(6)-O(26)	79.2(3)	O(110)-Tb(13)-O(104)	135.67(18)
O(28)-Gd(6)-O(26)	135.2(4)	O(118)-Tb(13)-O(104)	78.61(17)
O(27)-Gd(6)-O(26)	54.6(3)	O(100)-Tb(13)-O(104)	140.01(17)
O(21)-Gd(6)-O(26)	140.1(3)	O(109)-Tb(13)-O(104)	82.92(17)
O(25)-Gd(6)-O(33)	103.0(4)	O(110)-Tb(13)-O(112)	90.70(17)
O(28)-Gd(6)-O(33)	91.5(4)	O(118)-Tb(13)-O(112)	85.83(17)
O(27)-Gd(6)-O(33)	84.0(4)	O(100)-Tb(13)-O(112)	121.43(16)
O(21)-Gd(6)-O(33)	76.4(3)	O(109)-Tb(13)-O(112)	162.39(17)
O(26)-Gd(6)-O(33)	84.2(3)	O(104)-Tb(13)-O(112)	82.62(17)

O(25)-Gd(6)-O(39)	85.0(4)	O(110)-Tb(13)-O(105)	80.81(18)
O(28)-Gd(6)-O(39)	90.6(4)	O(118)-Tb(13)-O(105)	132.46(17)
O(27)-Gd(6)-O(39)	79.3(4)	O(100)-Tb(13)-O(105)	151.19(17)
O(21)-Gd(6)-O(39)	121.0(3)	O(109)-Tb(13)-O(105)	83.84(17)
O(26)-Gd(6)-O(39)	82.1(3)	O(104)-Tb(13)-O(105)	54.87(18)
O(39)-Gd(6)-O(33)	162.6(4)	O(112)-Tb(13)-O(105)	79.63(17)
O(25)-Gd(6)-O(38)	74.1(3)	O(110)-Tb(13)-O(113)	75.23(17)
O(28)-Gd(6)-O(38)	75.3(4)	O(118)-Tb(13)-O(113)	74.90(17)
O(27)-Gd(6)-O(38)	125.0(3)	O(100)-Tb(13)-O(113)	69.06(15)
O(21)-Gd(6)-O(38)	68.7(3)	O(109)-Tb(13)-O(113)	144.63(16)
O(26)-Gd(6)-O(38)	128.5(3)	O(104)-Tb(13)-O(113)	128.81(16)
O(33)-Gd(6)-O(38)	144.1(3)	O(112)-Tb(13)-O(113)	52.73(16)
O(39)-Gd(6)-O(38)	52.8(3)	O(105)-Tb(13)-O(113)	125.27(16)
C(1)-O(2)-Gd(1)	90.0(10)	C(1)-O(2)-Tb(1)	91.3(5)
C(1)-O(3)-Gd(1)	92.0(10)	C(1)-O(3)-Tb(1)	91.4(5)
C(12)-O(4)-Gd(1)	95.6(9)	C(34)-O(8)-Tb(1)	164.0(5)
C(12)-O(5)-Gd(1)	90.2(8)	C(45)-O(10)-Tb(1)	131.6(5)
C(56)-O(12)-Gd(1)	137.9(11)	C(78)-O(16)-Tb(1)	87.5(5)
C(67)-O(14)-Gd(1)	127.2(11)	C(78)-O(17)-Tb(1)	98.6(4)
C(78)-O(16)-Gd(1)	155.2(10)	C(89)-O(19)-Tb(1)	142.5(5)
C(34)-O(9)-Gd(2)	125.5(11)	C(12)-O(4)-Tb(2)	92.0(4)
C(45)-O(10)-Gd(2)	94.1(10)	C(12)-O(5)-Tb(2)	91.3(4)
C(45)-O(11)-Gd(2)	92.9(11)	C(34)-O(8)-Tb(2)	90.1(4)
C(67)-O(15)-Gd(2)	139.8(11)	C(34)-O(9)-Tb(2)	97.4(4)
C(78)-O(16)-Gd(2)	91.5(9)	C(45)-O(11)-Tb(2)	138.1(5)
C(78)-O(17)-Gd(2)	96.3(10)	C(56)-O(12)-Tb(2)	127.6(5)
C(89)-O(18)-Gd(2)	164.5(13)	C(67)-O(15)-Tb(2)	157.2(5)
C(12)-O(5)-Gd(3)	163.6(10)	C(23)-O(6)-Tb(3)	90.4(5)
C(23)-O(6)-Gd(3)	92.1(11)	C(23)-O(7)-Tb(3)	94.2(5)
C(23)-O(7)-Gd(3)	91.6(9)	C(56)-O(13)-Tb(3)	139.8(5)
C(34)-O(8)-Gd(3)	140.2(11)	C(67)-O(14)-Tb(3)	96.7(5)
C(56)-O(13)-Gd(3)	132.0(10)	C(67)-O(15)-Tb(3)	92.0(4)
C(89)-O(18)-Gd(3)	89.0(11)	C(78)-O(16)-Tb(3)	163.6(5)
C(89)-O(19)-Gd(3)	97.5(9)	C(89)-O(18)-Tb(3)	126.1(5)
C(101)-O(22)-Gd(4)	92.1(11)	C(101)-O(102)-Tb(11)	91.9(4)
C(101)-O(23)-Gd(4)	89.8(11)	C(101)-O(103)-Tb(11)	91.6(4)
C(112)-O(24)-Gd(4)	93.3(9)	C(134)-O(108)-Tb(11)	143.2(5)
C(112)-O(25)-Gd(4)	89.6(9)	C(167)-O(115)-Tb(11)	128.6(4)
C(156)-O(32)-Gd(4)	144.3(11)	C(178)-O(117)-Tb(11)	164.1(5)
C(167)-O(34)-Gd(4)	130.1(10)	C(189)-O(118)-Tb(11)	91.0(4)
C(178)-O(36)-Gd(4)	162.2(13)	C(189)-O(119)-Tb(11)	96.7(4)
C(134)-O(29)-Gd(5)	131.6(10)	C(123)-O(106)-Tb(12)	93.0(5)
C(145)-O(30)-Gd(5)	91.4(11)	C(123)-O(107)-Tb(12)	91.2(4)
C(145)-O(31)-Gd(5)	91.5(8)	C(145)-O(111)-Tb(12)	131.5(5)
C(167)-O(35)-Gd(5)	138.4(10)	C(156)-O(113)-Tb(12)	163.6(5)
C(178)-O(36)-Gd(5)	92.3(11)	C(167)-O(114)-Tb(12)	140.3(5)
C(178)-O(37)-Gd(5)	99.4(11)	C(178)-O(116)-Tb(12)	97.8(4)
C(189)-O(38)-Gd(5)	164.1(10)	C(178)-O(117)-Tb(12)	88.9(4)
C(112)-O(25)-Gd(6)	157.2(10)	C(112)-O(104)-Tb(13)	91.9(4)
C(123)-O(26)-Gd(6)	92.0(8)	C(112)-O(105)-Tb(13)	91.2(4)
C(123)-O(27)-Gd(6)	91.4(9)	C(134)-O(109)-Tb(13)	119.9(5)
C(134)-O(28)-Gd(6)	138.7(12)	C(145)-O(110)-Tb(13)	139.2(5)
C(156)-O(33)-Gd(6)	115.4(11)	C(156)-O(112)-Tb(13)	97.4(4)
C(189)-O(38)-Gd(6)	88.0(9)	C(156)-O(113)-Tb(13)	89.2(4)
C(189)-O(39)-Gd(6)	95.2(9)	C(189)-O(118)-Tb(13)	158.1(5)
O(3)-C(1)-O(2)	123.0(15)	O(2)-C(1)-O(3)	121.8(8)
O(5)-C(12)-O(4)	121.1(14)	O(5)-C(12)-O(4)	120.8(7)
O(6)-C(23)-O(7)	120.1(16)	O(6)-C(23)-O(7)	120.3(7)
O(9)-C(34)-O(8)	126.9(15)	O(9)-C(34)-O(8)	119.9(6)
O(11)-C(45)-O(10)	118.7(17)	O(10)-C(45)-O(11)	125.2(7)
O(13)-C(56)-O(12)	125.1(16)	O(12)-C(56)-O(13)	125.5(7)

O(15)-C(67)-O(14)	125.2(16)	O(14)-C(67)-O(15)	118.6(7)
O(17)-C(78)-O(16)	118.6(14)	O(17)-C(78)-O(16)	120.6(7)
O(18)-C(89)-O(19)	121.1(17)	O(18)-C(89)-O(19)	124.3(7)
O(22)-C(101)-O(23)	121.6(17)	O(103)-C(101)-O(102)	121.2(7)
O(25)-C(112)-O(24)	123.3(15)	O(105)-C(112)-O(104)	120.9(6)
O(26)-C(123)-O(27)	121.3(13)	O(107)-C(123)-O(106)	120.5(7)
O(28)-C(134)-O(29)	126.1(17)	O(109)-C(134)-O(108)	124.2(7)
O(31)-C(145)-O(30)	121.2(15)	O(111)-C(145)-O(110)	125.2(7)
O(32)-C(156)-O(33)	123.5(16)	O(112)-C(156)-O(113)	120.6(6)
O(35)-C(167)-O(34)	126.0(14)	O(115)-C(167)-O(114)	125.3(6)
O(36)-C(178)-O(37)	116.4(18)	O(116)-C(178)-O(117)	120.4(7)
O(38)-C(189)-O(39)	123.8(15)	O(119)-C(189)-O(118)	119.3(6)

3- Electrochemistry

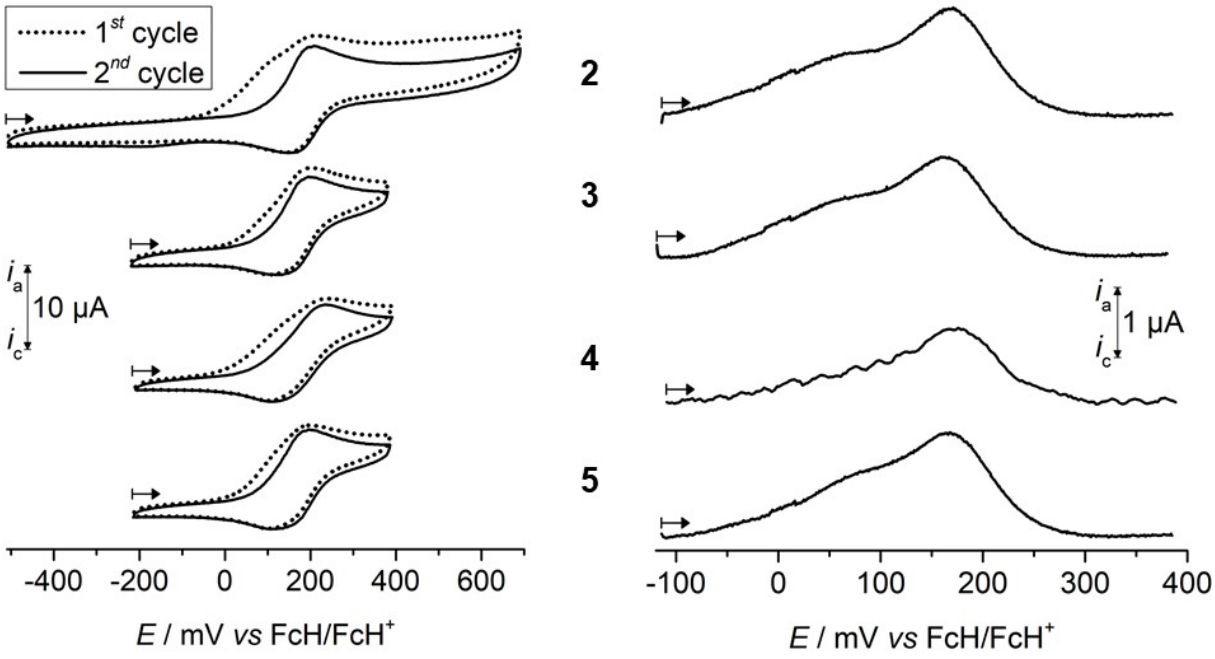


Figure S10. Cyclic voltammograms (scan rate 100 mV·s^{-1}; left) and respective square wave voltammograms (duration: 1 s, amplitude: 5 mV, pulse: 25 mV; right) of **2** – **5**; The experiments were performed in a dimethylformamide solution of analyte (0.25 mmol·L^{-1}) at 25 °C using 0.1 mol·L^{-1} [Bu_4N][ClO_4] as supporting electrolyte and potentials given *vs* ferrocene/ferrocenium.

Table S7. Cyclic voltammetry data of **2** – **5**.[a)]

Compoud	E_{pc} / mV[b)]	$E°'$ / mV[c)] (ΔE_p / mV)[d)]
2	-210	180 (80)
3	-260	185 (81)
4	-260	185 (80)
5	-210	175 (78)

a) Pontentials *vs* FcH/FcH$^+$ (scan rate 100 mV·s^{-1}) at a glassy carbon electrode of 0.25 mmol·L^{-1} solutions of analyte in dimethylformamide containing 0.1 mol·L^{-1} of [Bu_4N][ClO_4] as supporting electrolyte at 25 °C. b) E_{pc} irreversible process. c) $E°'$ = formal potential. d) ΔE_p = difference between the cathodic and anodic peak potentials $|E_{pc} - E_{pa}|$.

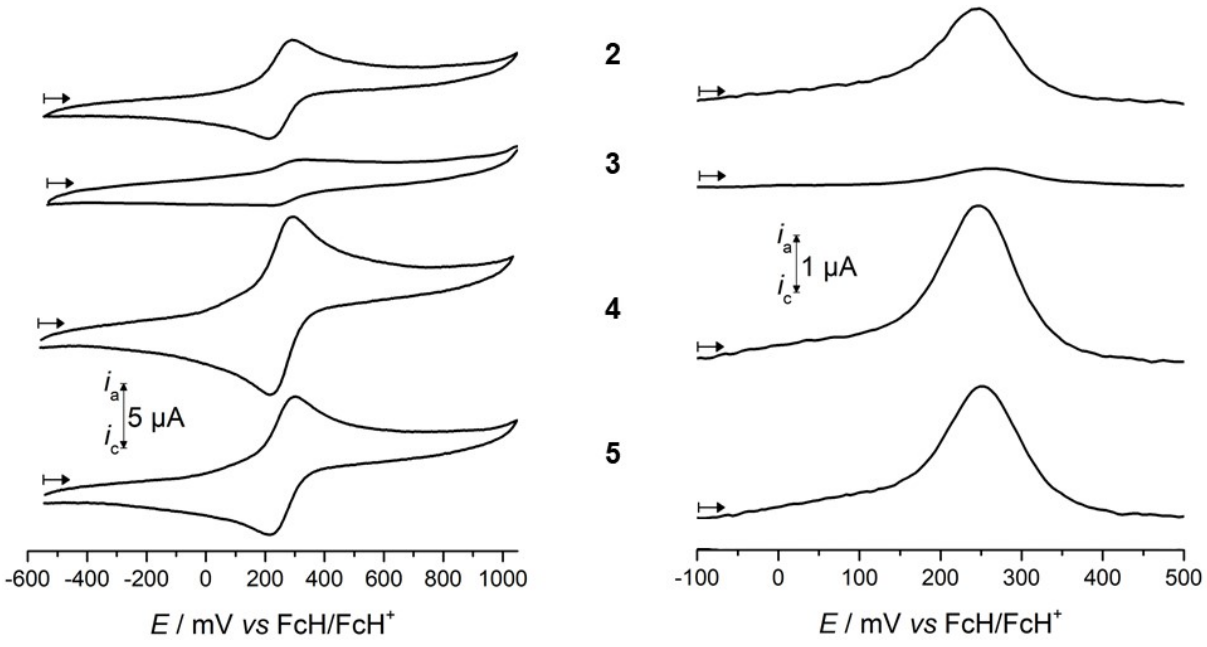


Figure S11. Cyclic voltammograms (scan rate 100 $mV \cdot s^{-1}$; left) and respective square wave voltammograms (duration: 1 s, amplitude: 5 mV, pulse: 25 mV; right) of **2** – **5**; The experiments were performed in a CH_2Cl_2 solution of conc. analyte (< 0.25 $mmol \cdot L^{-1}$) at 25 °C using 0.1 $mol \cdot L^{-1}$ $[Bu_4N][B(C_6F_5)_4]$ as supporting electrolyte and potentials given *vs* ferrocene/ferrocenium.

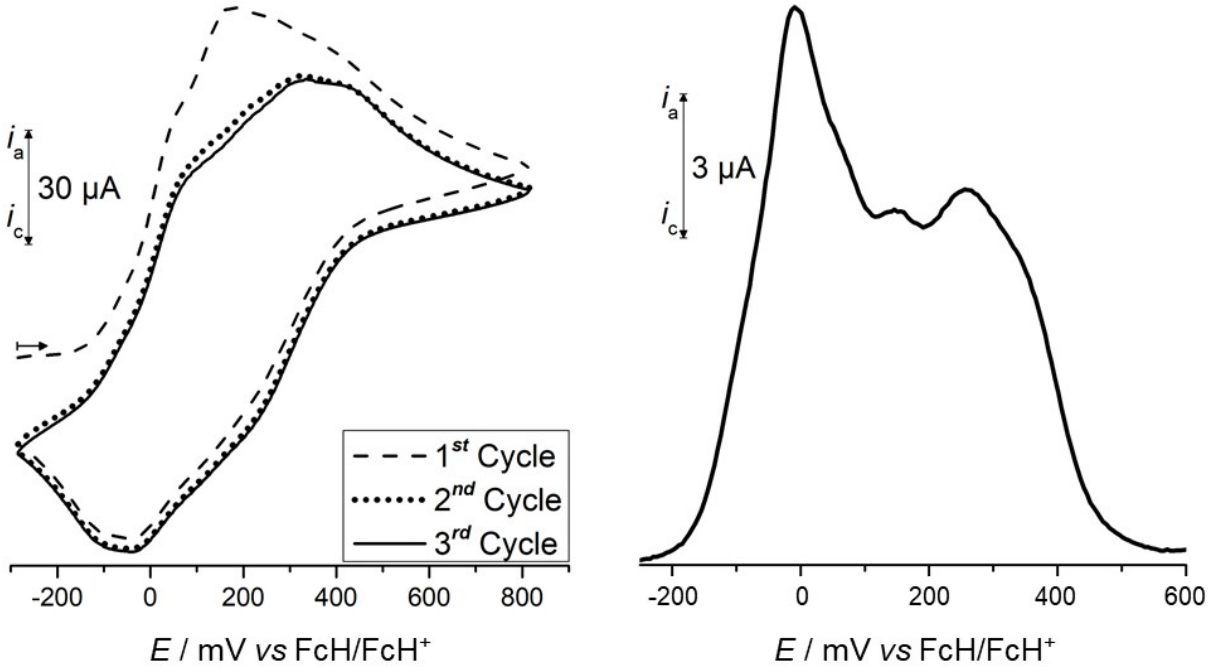


Figure S12. Cyclic voltammogram (left) and the respective square wave voltammogram (duration: 1 s, amplitude: 5 mV, pulse: 25 mV) (right) of **7**; Both experiments were performed in a CH_2Cl_2 solution of analyte (1.0 $mmol \cdot L^{-1}$) at 25 °C using 0.1 $mol \cdot L^{-1}$ $[Bu_4N][B(C_6F_5)_4]$ as supporting electrolyte and potentials given *vs* ferrocene/ferrocenium.

4- Computational Chemistry

Table S8. Effective ion radii (pm) of **Gd** and **Tb** compared with **Y** and La for various coordination numbers.[1]

Coordination number	r **Y** / pm	Δr / pm	r **Gd** / pm	Δr / pm	r **La** / pm
6	104	3.8	107.8	9.4	117.2
7	110	4	114	10	124
8	115.9	3.4	119.3	10.7	130
9	121.5	3.2	124.7	10.9	135.6
	r **Y** / pm		r **Tb** / pm		r **La** / pm
6	104	2.3	106.3	10.9	117.2
7	110	2	112	12	124
8	115.9	2.1	118	12	130
9	121.5	2	123.5	12.1	135.6

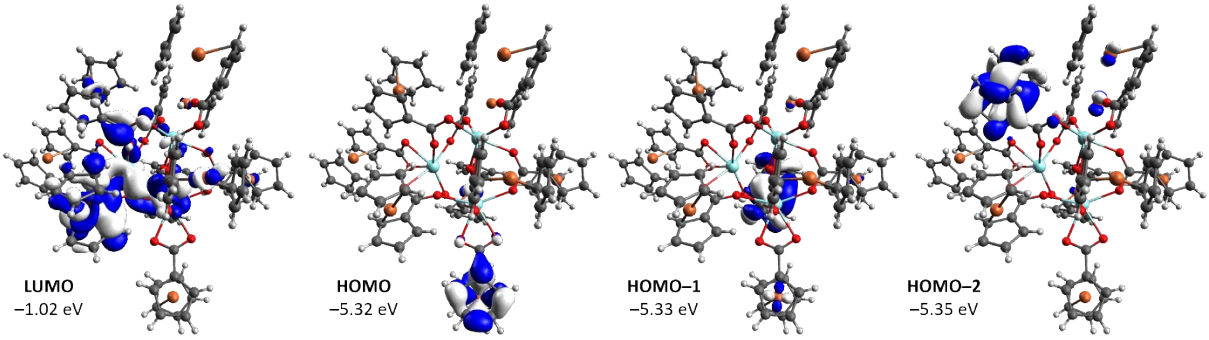


Figure S13. Plots of the frontier orbitals (contours plotted at ±0.02 $(e/bohr^3)^{1/2}$) and their energies of $\mathbf{Y}_t$ (B3LYP, def2-TZVP, def2/J, CPCM (CH_2Cl_2)) considering a 180 ° rotation of the first (bottom) fragment.

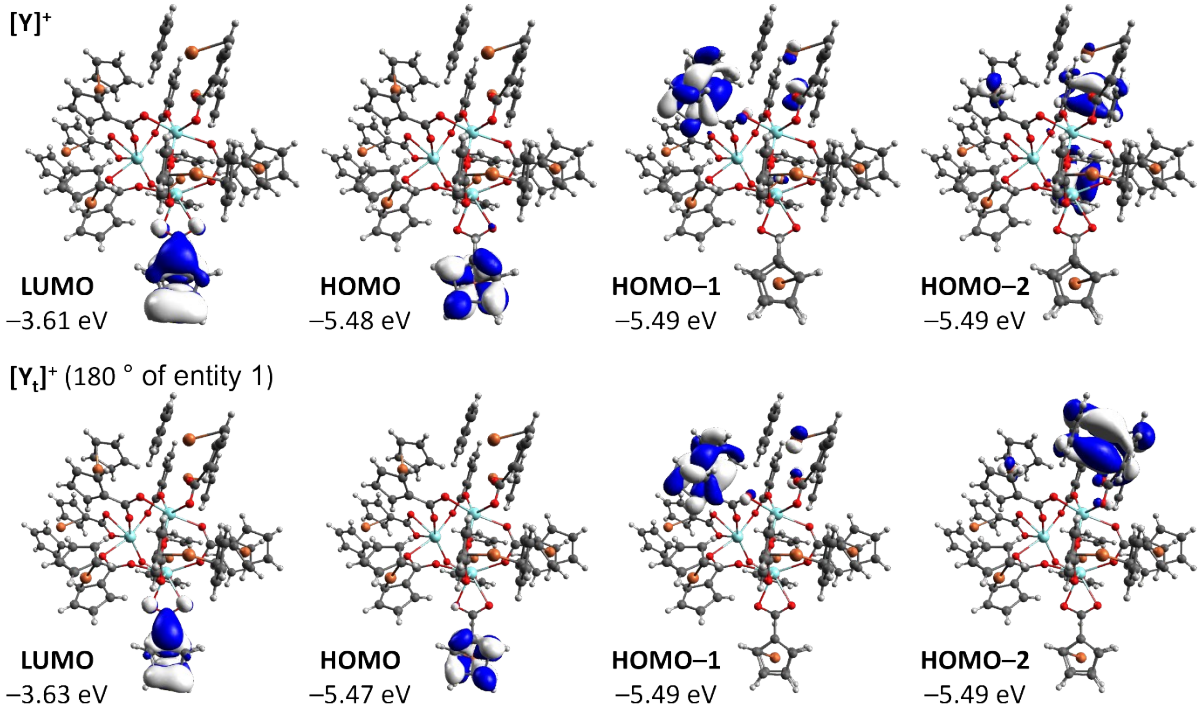


Figure S14. Plots of the β-frontier orbitals (contours plotted at ±0.02 $(e/bohr^3)^{1/2}$) and their energies of $[\mathbf{Y}]^+$ (top) and $[\mathbf{Y_t}]^+$ (bottom) (B3LYP, def2-TZVP, def2/J, CPCM (CH_2Cl_2)) considering a 180 ° rotation of the first (bottom) fragment.

Second molecule in the asymmetric unit

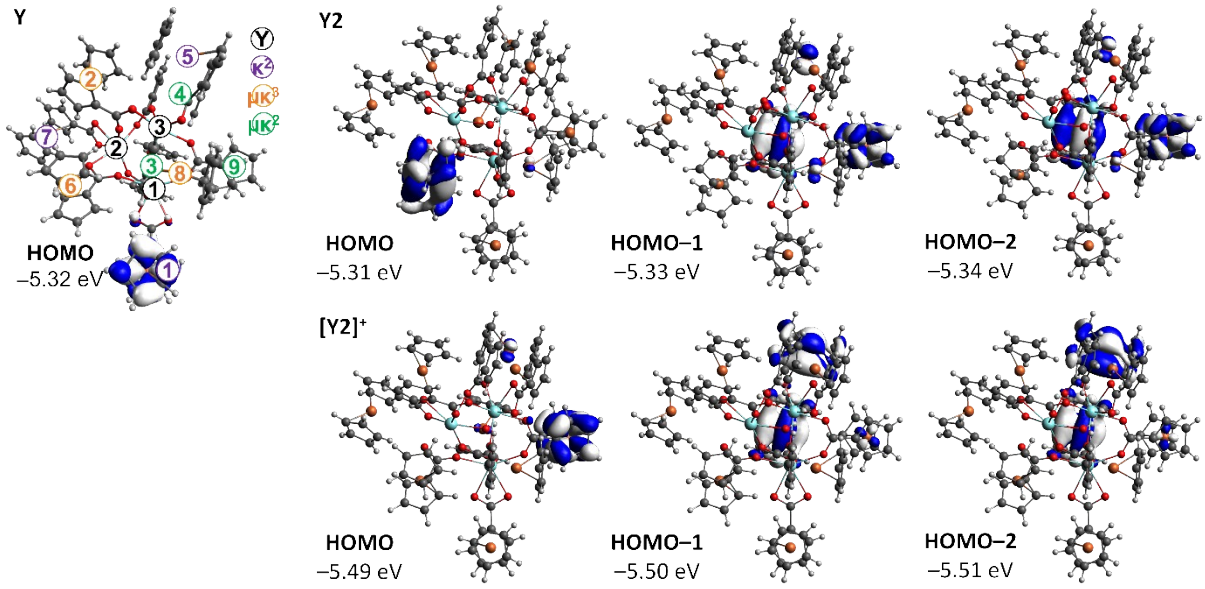


Figure S15. Plots of the (α-)frontier orbitals (contours plotted at ±0.02 $(e/bohr^3)^{1/2}$) and their energies of **Y2** and its single-oxidized form $[\mathbf{Y2}]^+$ (the second molecule in the asymmetric unit) (B3LYP, def2-TZVP, def2/J, CPCM (CH_2Cl_2)).

Table S9. Crystallographic data and structure refinement details for compounds **2** – **5**.

		2	**3**	**4**	**5**
CCDC		2248459	2248460	2248461	2248462
Empirical formula		$C_{78}H_{86}Fe_6N_4O_{18}Sm_2$	$C_{78}H_{86}Eu_2Fe_6N_4O_{18}$	$C_{78}H_{86}Fe_6Gd_2N_4O_{18}$	$C_{78}H_{86}Fe_6N_4O_{18}Tb_2$
Formula mass ($g \cdot mol^{-1}$)		2003.30	2006.52	2017.10	2020.44
Temperature (K)		120	120	100	120
Wavelength (Å)		1.54184	1.54184	1.54184	1.54184
Crystal system		Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group		$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
Unit cell dimensions (Å, °)	*a*	14.7209(5)	14.7146(2)	14.6899(5)	14.6912(2)
	b	11.9096(3)	11.9172(2)	11.9110(5)	11.9184(1)
	c	22.3766(8)	22.3816(3)	22.3609(9)	22.3365(2)
	α	90	90	90	90
	β	106.077(4)	105.931(2)	105.911(4)	105.982(1)
	γ	90	90	90	90
V ($Å^3$)		3769.6(2)	3774.03(10)	3762.6(3)	3759.85(7)
Z		2	2	2	2
D_{calc} ($Mg \cdot m^{-3}$)		1.765	1.766	1.780	1.785
Absorption coefficient (mm^{-1})		21.075	21.263	20.796	18.651
F(000)		2012	2016	2020	2024
θ range for data collection (°)		3.124 to 65.983	3.123 to 66.415	3.128 to 72.350	3.129 to 65.992
Limiting indices		-16 ≤ *h* ≤ 17, -8 ≤ *k* ≤ 14, -26 ≤ *l* ≤ 25	-17 ≤ *h* ≤ 15, -13 ≤ *k* ≤ 13, -16 ≤ *l* ≤ 26	-18 ≤ *h* ≤ 17, -14 ≤ *k* ≤ 11, -27 ≤ *l* ≤ 19	-17 ≤ *h* ≤ 17, -13 ≤ *k* ≤ 14, -21 ≤ *l* ≤ 26
Reflections collected		16313	12567	14950	19070
Reflections unique / R_{int}[a)]		6536 / 0.0477	6516 / 0.0347	7264 / 0.0554	6478 / 0.0331
Max. and min. transmission		1.00000 and 0.16766	1.00000 and 0.55597	1.00000 and 0.07629	1.00000 and 0.38114
Data / restraints / parameters		6536 / 5 / 385	6516 / 2 / 499	7264 / 3 / 493	6478 / 2 / 499
Goodness–of–fit on F^2[b)]		1.083	1.008	1.026	1.016
Final *R* indices [$I>2\sigma(I)$][c)]		R_1 = 0.0489, wR_2 = 0.1215	R_1 = 0.0303, wR_2 = 0.0631	R_1 = 0.0480, wR_2 = 0.1202	R_1 = 0.0272, wR_2 = 0.0647
R indices (all data)[c)]		R_1 = 0.0593, wR_2 = 0.1275	R_1 = 0.0397, wR_2 = 0.0660	R_1 = 0.0583, wR_2 = 0.1277	R_1 = 0.0327, wR_2 = 0.0667
Largest diff. peak / hole ($e \cdot Å^{-3}$)		2.123 / -1.622	1.303 / -0.534	1.693 / -1.007	0.934 / -0.558

a) $R_{int} = \sum \left| F_0^2 - F_0^2(mean) \right| / \sum F_0^2$; where $F_0^2(mean)$ is the average intensity of symmetry equivalent diffractions.

b) $S = \left[\sum w(F_0^2 - F_c^2)^2 \right] / (n-p)^{1/2}$; where *n* = number of reflections, *p* = number of parameters.

[c] $R = \sum(|F_0| - |F_c|)/\sum|F_0|$, $wR = \left[\sum(w(F_0^2 - F_c^2)^2)/\sum(wF_0^4)\right]^{1/2}$

Table S10. Crystallographic data and structure refinement details for compounds **6** and **7**.

		{**6**·[NBu_4]Cl}$_2$	{**7**·[NBu_4]Cl·Et_2O·THF}$_2$
CCDC		2248463	2248464
Empirical formula		$C_{131}H_{154}ClFe_9Gd_3N_2O_{19}$ [+ solvent + [NBu_4]Cl]	$C_{1094}H_{1318}Cl_8Fe_{72}N_{16}O_{163}Tb_{24}$
Moiety Formula		$C_{99}H_{82}Fe_9Gd_3O_{19}$, 2($C_{16}H_{36}N$), Cl [+ solvent + [$NBu_4$]Cl]	25418.45
Formula mass (g·mol^{-1})		3070.40 [+ solvent + [NBu_4]Cl]	
Temperature (K)		120	100
Wavelength (Å)		1.54184	0.71073
Crystal system		Monoclinic	Monoclinic
Space group		$P2_1/n$	$P2_1/n$
Unit cell dimensions (Å, °)	*a*	15.2698(6)	15.2447(10)
	b	42.9380(2)	43.0160(3)
	c	47.5450(2)	47.3890(3)
	α	90	90
	β	90.118(4)	90.239(2)
	γ	90	90
V (Å^3)		31173(2)	31076(4)
Z		8	1
D_{calc} (Mg·m^{-3})		1.308	1.358
Absorption coefficient (mm^{-1})		15.173	2.231
F(000)		12392	12866
θ range for data collection (°)		3.072 to 65.000	2.596 to 25.000
Limiting indices		-16 ≤ *h* ≤ 17, -50 ≤ *k* ≤ 50, -46 ≤ *l* ≤ 55	-18 ≤ *h* ≤ 18, -51 ≤ *k* ≤ 51, -56 ≤ *l* ≤ 56
Reflections collected		118715	266802
Reflections unique / R_{int}[a)]		52855 / 0.1708	54494 / 0.0524
Max. and min. transmission		1.00000 and 0.31155	0.99999 and 0.34871
Data / restraints / parameters		52855 / 5106 / 2687	54494 / 5353 / 3161
Goodness–of–fit on F^2[b)]		0.803	1.117
Final *R* indices [$I>2\sigma(I)$][c)]		R_1 = 0.0893, wR_2 = 0.1778	R_1 = 0.0669, wR_2 = 0.1422
R indices (all data)[c)]		R_1 = 0.2207, wR_2 = 0.2415	R_1 = 0.0758, wR_2 = 0.1459
Largest diff. peak / hole (e·Å^{-3})		1.054 / -1.099	4.414 / -2.988
Squeeze data		8634.4 Å^3; 1908 e$^-$/cell	5383.4 Å^3; 1693.6 e$^-$/cell

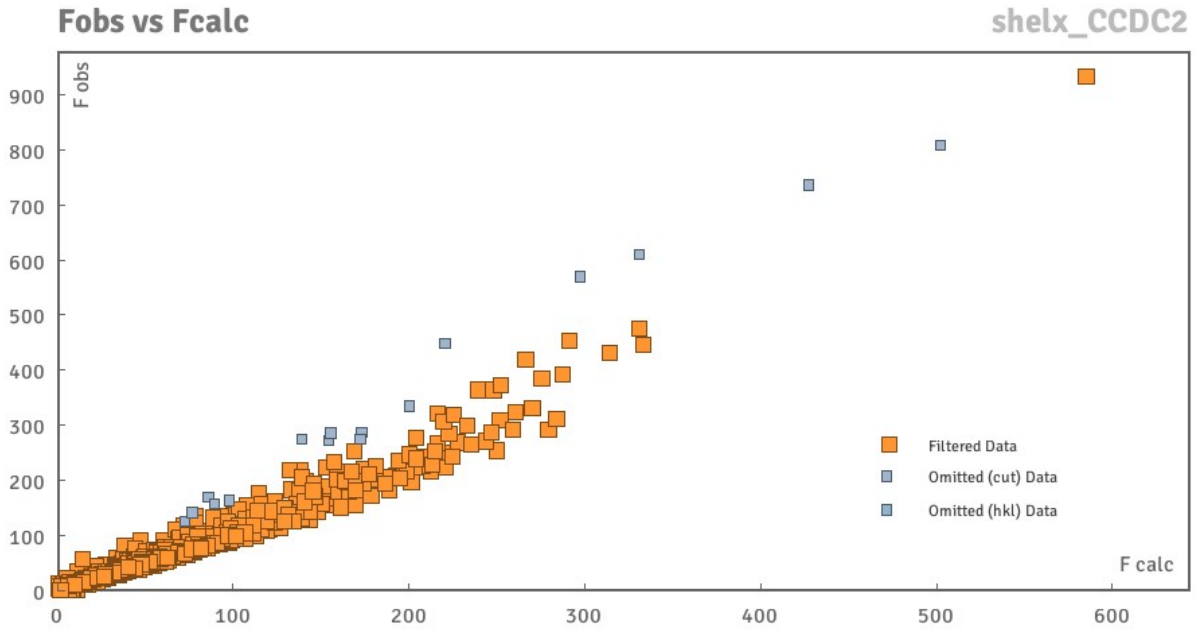
a) $R_{int} = \sum\left|F_0^2 - F_0^2(mean)\right| / \sum F_0^2$; where $F_0^2(mean)$ is the average intensity of symmetry equivalent diffractions.

b) $S = \left[\sum w(F_0^2 - F_c^2)^2\right] / (n-p)^{1/2}$; where *n* = number of reflections, *p* = number of parameters.

c) $R = \sum(|F_0| - |F_c|) / \sum|F_0|$, $wR = \left[\sum(w(F_0^2 - F_c^2)^2) / \sum(wF_0^4)\right]^{1/2}$

Miscellaneous

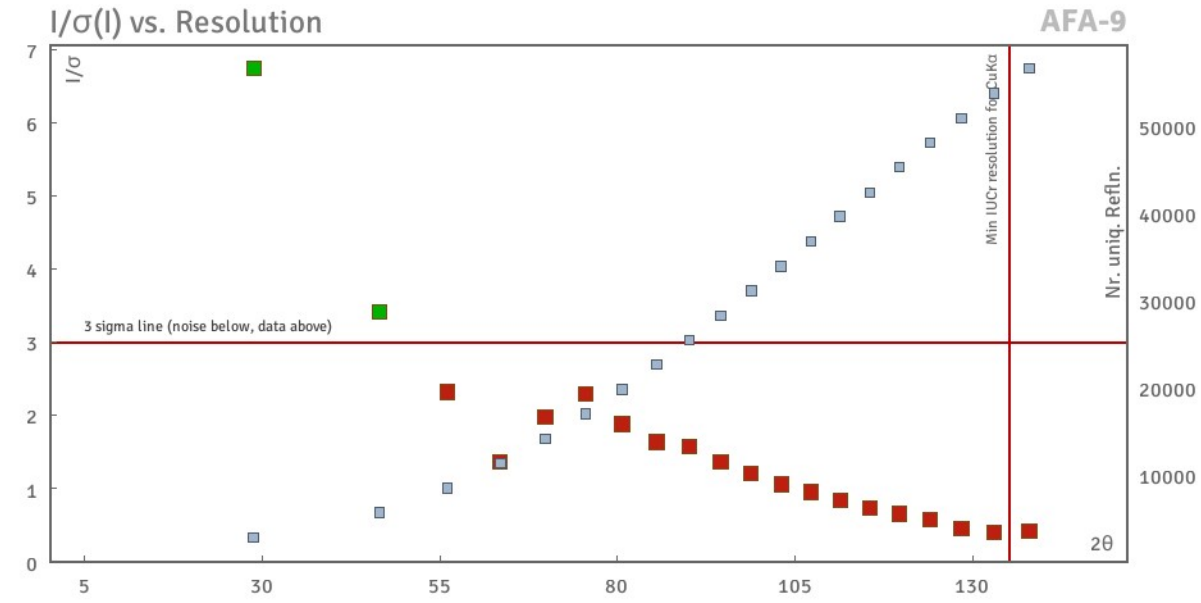
In case of compound **2** we could not perform a proper face absorption correction as we did not measure a crystal movie. The crystallographic reviewer asked for a potential re-measurement, which we could not do as well as it was not possible to obtain sufficiently large crystals. On request of this referee we should add here two graphs:

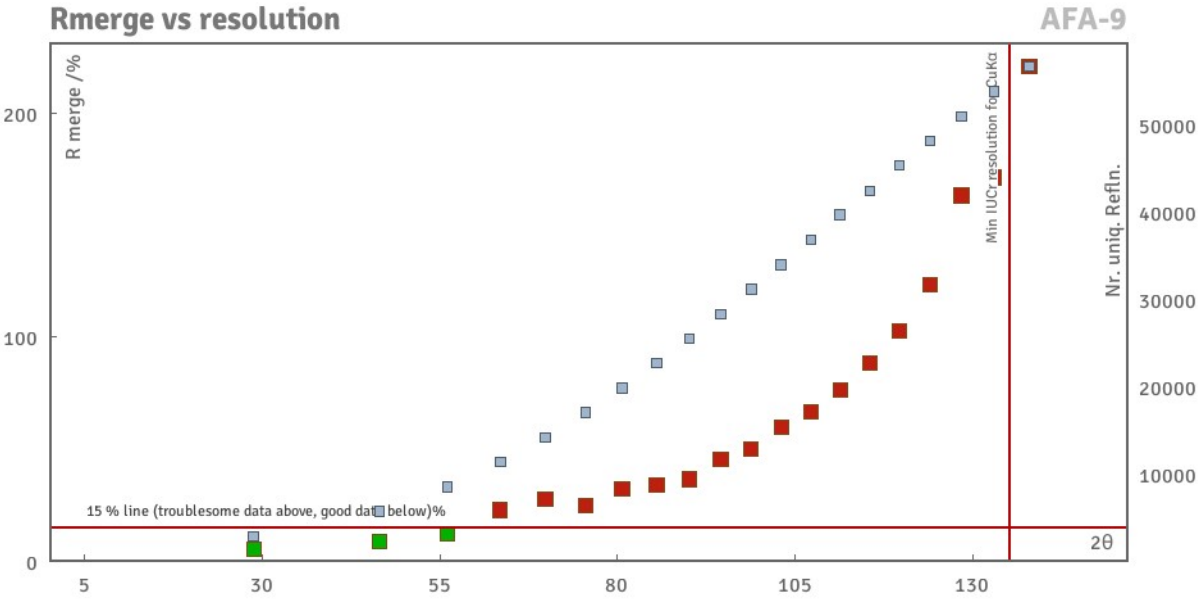


Reviewer comment: " … At the very least, please perform a proper face absorption correction. If you can not do this, then please add the attached graph to the SI, together with an explanation why it is impossible to recollect new data and/or perform a face absorption correction. … "

Compound **6** and **7** are isomorph. While in case of compound **7** comparatively large crystals could be obtained, allowing measurement with Mo Ka radiation, in case of **6** the crystal were much smaller. Furthermore, already **7** did possess a large VOID volume, although several packing solvent molecules could be refined. In case **6**, however, not. From our point of view missing packing solvents molecules and/or disordered one lead to a very weak diffractivity of the crystals **6**. Further information are given in the manuscript and in the .cif files as well.

Reviewe comment: " **If you wish to publish this structure, please report the contents of the mask properly and add the attached graphs to your SI together with a detailed explanation why it was impossible to obtain better data for this material. … "**





5- Reference

1 R. D. Shannon, *Acta Crystallogr. Sect. A*, 1976, **32**, 751–767.

[1] M. Llunell, D. Casanova, J. Cirera, P. Alemany, S. Alvarez, Shape 2.1 program package, 2013, University of Barcelona.