Supporting Information

Symmetry Related [$Dy^{III}_6Mn^{III}_{12}$] Cores with Different Magnetic Anisotropies

Jun-Liang Liu,[a] Fu-Sheng Guo,[a] Zhao-Sha Meng,[a] Yan-Zhen Zheng,[d] Ji-Dong Leng,[a] Ming-Liang Tong,*[a] Liviu Ungur,[b] Liviu F. Chibotaru,*[b] Katie J. Heroux[c] and David N. Hendrickson*[c]

[a] *Key Laboratory of Bioinorganic and Synthetic Chemistry of Ministry of Education, State Key Laboratory of Optoelectronic Materials and Technologies, School of Chemistry & Chemical Engineering, Sun Yat-Sen University, Guangzhou, 510275, P. R. China. Fax: (+)86 20 8411-2245; E-mail: tongml@mail.sysu.edu.cn*

[b] *Division of Quantum and Physical Chemistry and INPAC – Institute of Nanoscale Physics and Chemistry, Celestijnenlaan 200F, Katholieke Universiteit Leuven, B-3001, Belgium. E-mail: Liviu.Chibotaru@chem.kuleuven.be*

[c] *Division of Quantum and Physical Chemistry and INPAC – Institute of Department of Chemistry and Biochemistry-0358, University of California at San Diego, La Jolla, California, 92093-0358 , U.S.A. E-mail: dhendrickson@ucsd.edu*

[d] *Applied Chemistry Research Center, Frontier Institute of Science and Technology, Xi'an JiaoTong University, Xi'an 710049, China*

Experimental Section

Synthesis of **1**: A mixture of 2-hydroxy-5-methylisophthalaldehyde (33 mg, 0.2 mmol) and 2-aminoethanol (15 mg, 0.25 mmol) in MeCN / MeOH (8 / 8 mL) were stirred and heated at 80 ^{o}C for an hour and the solution turned dark yellow. It was then $DyCl_3 \cdot 6H_2O$ (38 mg, 0.1 mmol), $Mn(OAc)_2 \cdot 4H_2O$ (49 mg, 0.2 mmol) and triethylamine (30 mg, 0.3 mmol) were added in order. The resulting brown solution was stirred under ambient conditions for more than 2 hours and then filtered. Small black crystals of **1** (~6% yield) were obtained until the solution nearly dried. Elemental analysis Calcd (%) for **1** (4873.09): C, 29.58; H, 4.05; N, 2.30. Found: C, 28.87; H, 4.12; N, 2.43. Infra-red (KBr disc, cm^{-1}): 3423s, 2930m, 2868m, 1677s, 1636vs, 1547vs, 1448vs, 1319m, 1232m, 1165w, 1050m, 974w, 864w, 836w, 766w, 620s, 541s.

Synthesis of **2**: 2-hydroxy-5-methylisophthalaldehyde (33 mg, 0.2 mmol) and 2-aminoethanol (12 mg, 0.2 mmol) in MeCN / MeOH (8 / 8 mL) were mixed at room temperature. It was then $LnCl_3 \cdot 6H_2O$ (0.1 mmol), $Mn(OAc)_2 \cdot 4H_2O$ (49 mg, 0.2 mmol) and triethylamine (30 mg, 0.3 mmol) was immediately added in order. The resulting brown solution was stirred under ambient conditions for more than 2 hours and then filtered. Black prism crystals of **2** (~6% yield) were obtained until the solution nearly dried. Elemental analysis Calcd (%) for **2-Dy** (5105.33): C, 30.58; H, 4.19; N, 2.19. Found: C, 30.95; H, 4.18; N, 2.42. Infra-red (KBr disc, cm^{-1}): 3422s, 2926m, 2868m, 1676s, 1636vs, 1548vs, 1448vs, 1320m, 1290m, 1231s, 1166w, 1041m, 972m, 635s, 561s. Elemental analysis Calcd (%) for **2-Y** (4529.68): C, 35.00; H, 4.41; N, 2.47. Found: C, 34.94; H, 4.43; N, 2.53. Infra-red (KBr disc, cm-1): 3426s, 2925m, 2867m, 1677s, 1636vs, 1549vs, 1448vs, 1322m, 1291m, 1232m, 1167w, 1047m, 972w, 639s, 561s.

Crystal data of **1** at 150(2) K: $C_{120}H_{196}Dy_6Mn_{12}N_8O_{93}$, M_r = 4873.09 g mol^{-1}, orthorhombic, space group *Fddd*, a = 22.6849(12) Å, b = 37.2467(18) Å, c = 45.910(3) Å, V = 38792(4) $Å^3$, Z = 8, ρ = 1.535 g cm^{-3}, T = 150 K, μ = 3.105 mm^{-1}, $F(000)$ = 17720, $2\theta_{max}$ = 26.00°. S = 0.912.

Crystal data of **2-Dy** at 150(2) K: $C_{130}H_{212}Dy_6Mn_{12}N_8O_{99}$, M_r = 5105.33 g mol^{-1}, triclinic, space group *P*-1, a = 19.7904(5) Å, b = 21.4477(4) Å, c = 26.7375(6) Å, α = 95.344(1) Å, β = 97.864(1) Å, γ = 115.293(1) Å, V = 10017.8(4) $Å^3$, Z = 2, ρ = 1.660 g cm^{-3}, T = 150 K, μ = 3.024 mm^{-1}, $F(000)$ = 4962, $2\theta_{max}$ = 27.00°. S = 1.099.

Crystal data of **2-Y** at 150(2) K: $C_{132}H_{198}Y_6Mn_{12}N_8O_{90}$, M_r = 4529.68 g mol^{-1}, triclinic, space group *P*-1, a = 19.8997(9) Å, b = 21.3603(11) Å, c = 26.7219(12) Å, α = 95.0010(10) Å, β = 97.6260(10) Å, γ = 115.0900(10) Å, V = 10064.7(8) $Å^3$, Z = 2, ρ = 1.495 g cm^{-3}, T = 150 K, μ = 2.519 mm^{-1}, $F(000)$ = 4600, $2\theta_{max}$ = 27.00°. S = 0.854.

The disordered water and methanol molecules could not be modelled properly; thus, the program SQUEEZE, a part of the PLATON package of crystallographic software, was used to calculate the solvent disorder area and remove its contribution to the overall intensity data. A total of 490 parameters for **1**, 2084 parameters for **2-Dy** and 2056 parameters for **2-Y** were refined in the final least-squares cycle using 4007 reflections for **1**, 30764 reflections for **2-Dy** and 13897 reflections for **2-Y** with $I > 2\sigma(I)$ to yield R_1 and wR_2 of 0.0709 and 0.1748 for **1**, R_1 and wR_2 of 0.0530 and 0.1484 for **2-Dy** and R_1 and wR_2 of 0.0864 and 0.2213 for **2-Y**,respectively.

The intensity data were recorded on a Rigaku R-AXIS SPIDER IP diffractometer (Mo$K\alpha$, λ = 0.71073 Å) at 150(2) K. The structure was solved by direct methods, and all non-hydrogen atoms were refined anisotropically by least square on F^2 using the SHELXTL program. Hydrogen atoms on organic ligands were generated by the riding mode (G. M. Sheldrick, SHELXTL97, program for crystal structure refinement, University of Göttingen, Germany, 1997). CCDC-779464-65 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge *via* www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, UK; fax: (+44)1223-336-033; or deposit@ccdc.cam.ac.uk).

Magnetic measurements were performed using a Quantum Design MPMS XL-7 SQUID magnetometer. The susceptibility measurement was performed in the 300-2 K temperature range with an applied field of 500 Oe. For magnetization measurements, the samples were sealed in parafilm to avoid any orientation of the crystallites. Ac magnetic susceptibilities were obtained with 5 Oe ac fields at zero dc fields.

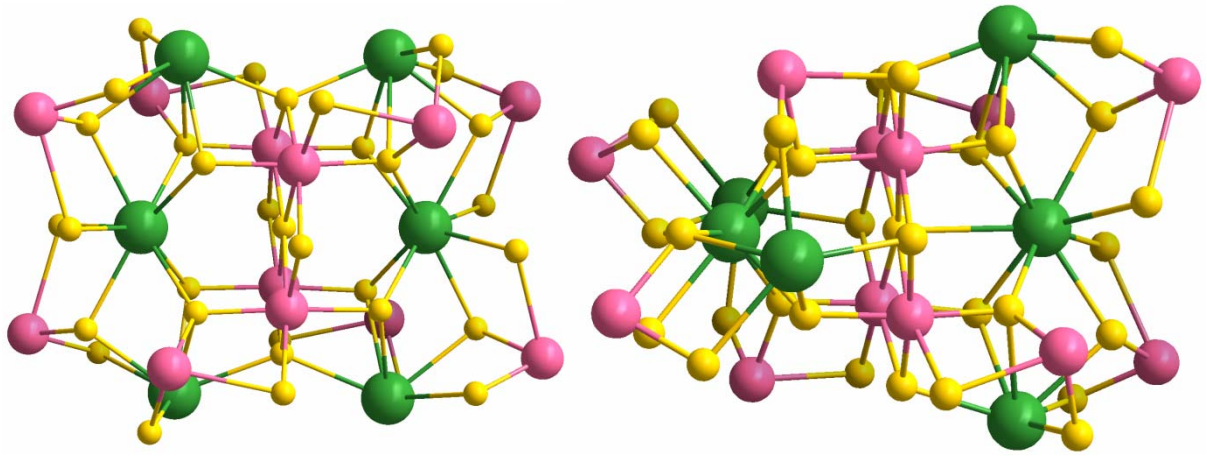

Figure S1. The cores of **1** (*left*) and **2** (*right*). Atom color code: Ln^{III} = green; Mn^{III} = magenta; O = yellow; N = blue.

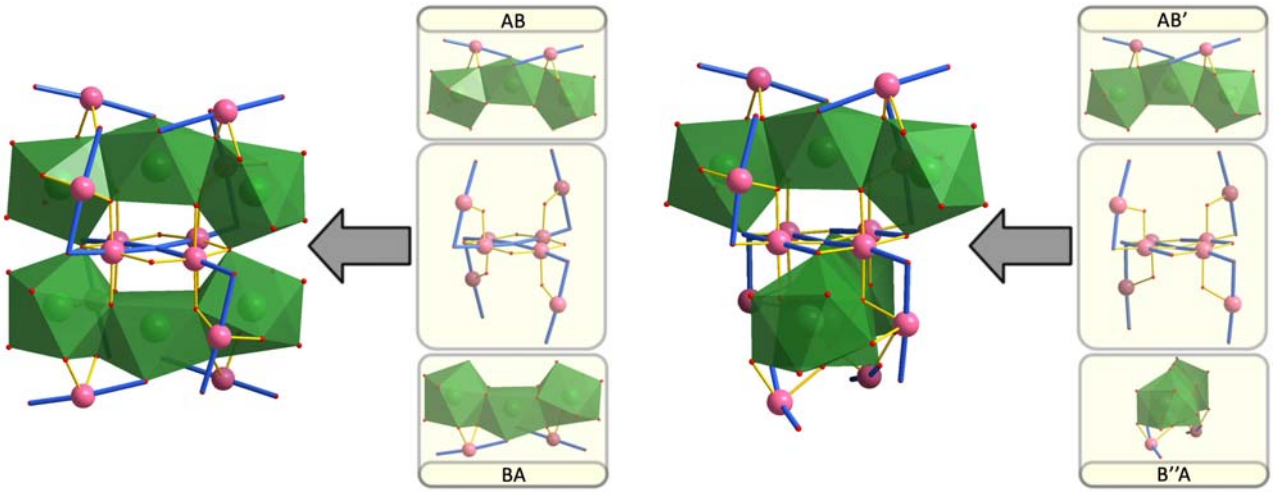

Figure S2. Composition of the $[Ln^{III}_6Mn^{III}_{12}]$ cores for **1** (*left*) and **2** (*right*). Each Ln^{III} is highlighted as a green polyhedron and the Jahn-Teller axes of Mn^{III} ions are highlighted as blue sticks. Hydrogen atoms and lattice solvent molecules have been omitted for clarity.

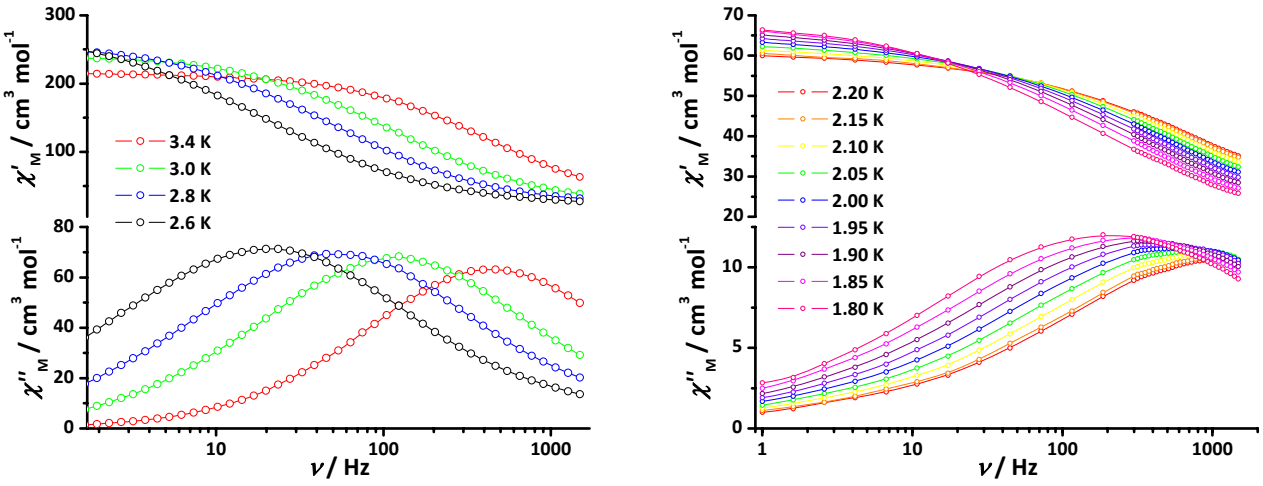

Figure S3. Variable-frequency ac susceptibility data for **1-Dy** (*left*) and **2-Dy** (*right*), collected at different temperatures under a zero dc field in a 5 G ac field.

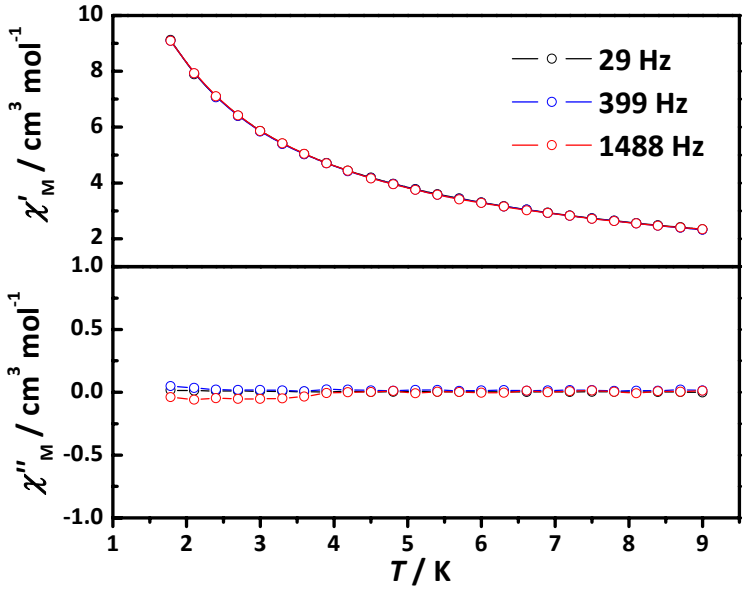

Figure S4. Plot of ac susceptibility vs. temperature for **2-Y** oscillating at 29-1488 Hz at H_{ac} = 5 G and H_{dc} = 0.

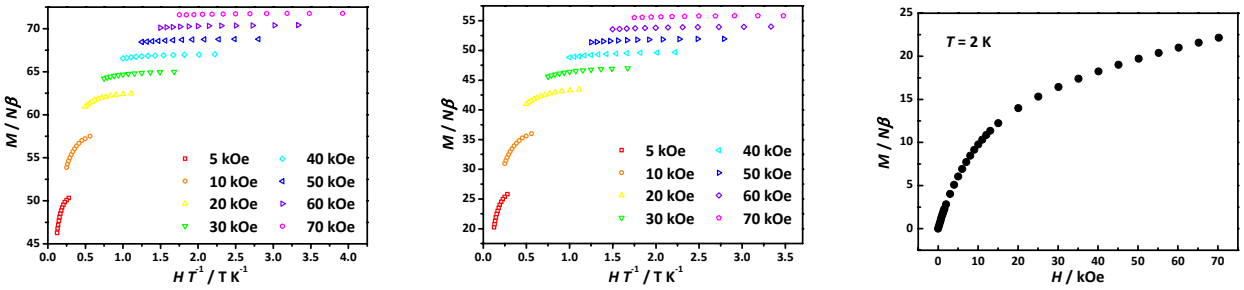

Figure S5. The plots of $M/N\beta$ vs. H/T for **1-Dy** (*left*) and **2-Dy** (*middle*), and $M/N\beta$ vs. H for **2-Y** (*right*) at 2 K.

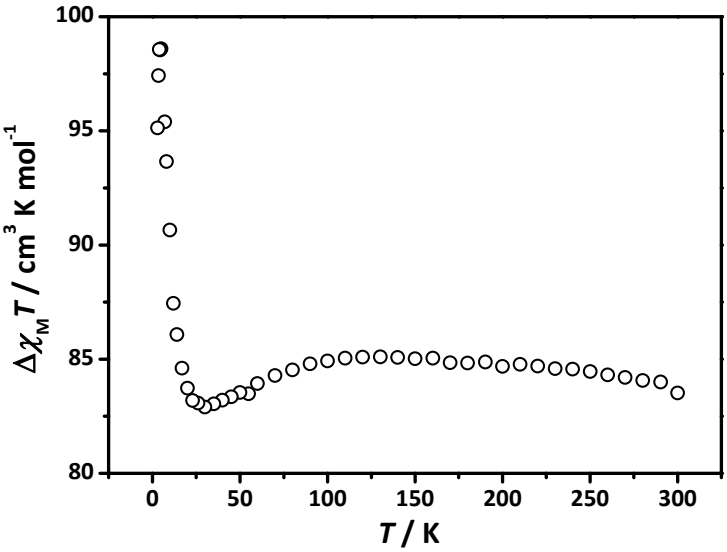

Figure S6. $\chi_m T$ vs T plots of subtracting **2-Y** from the plot **2-Dy**.

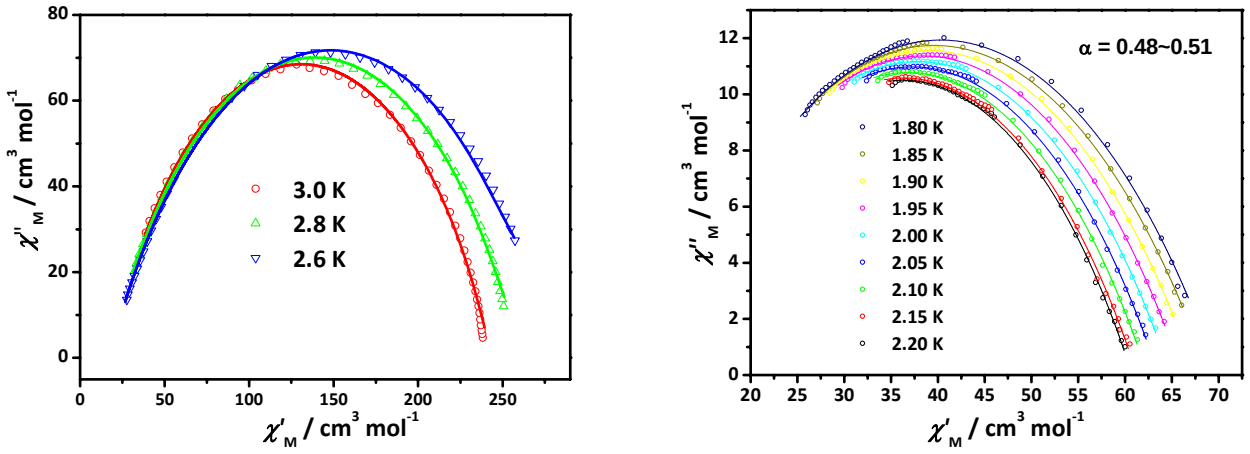

Figure S7. Cole-Cole plots for **1-Dy** (*left*) and **2-Dy** (*right*), obtained from variable-frequency ac susceptibility data under a zero dc field in the temperature range. Solid lines represent fits to the data using a generalized Debye model. The α parameters were abstracted, giving 0.30-0.36 for **1-Dy**, 0.48-0.51 for **2-Dy**, respectively.

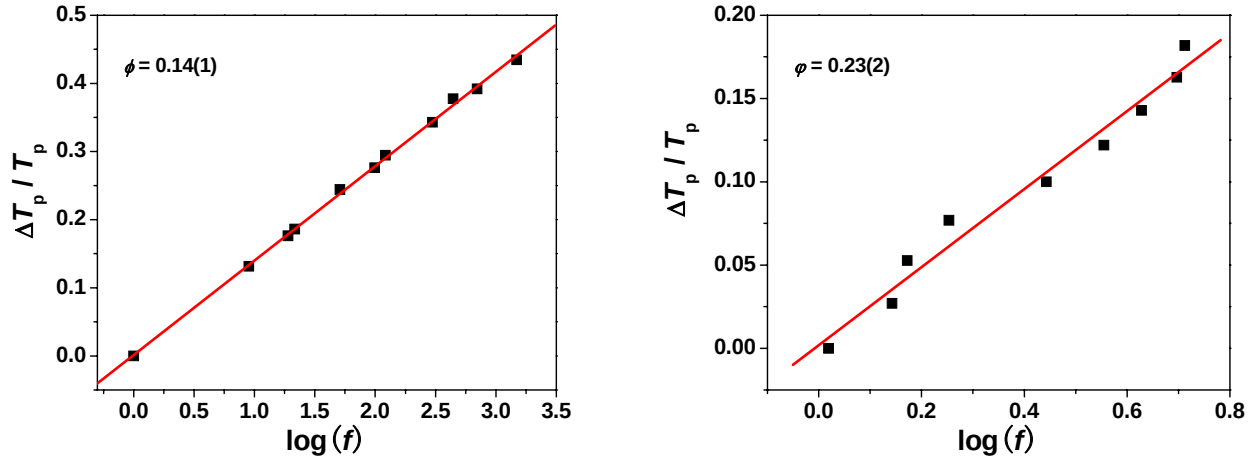

Figure S8. The log(*f*) vs. $\Delta T_p/T_p$ plots for **1-Dy** (*left*) and **2-Dy** (*right*). The value of φ can be extracted from the slope.

Table S1. Bond valence sum calculations of Mn and Ln oxidation states in the crystal structures of **1-Dy**, **2-Dy** and **2-Y**.

Complex **1-Dy**			
Dy1	2.976(24)	Dy2	2.644(19)
	+2	+3	+4
Mn1	3.547(29)	3.271(27)	3.209(27)
Mn2	3.439(38)	3.204(36)	2.941(34)
Mn3	3.556(40)	3.312(37)	3.080(36)

Complex **2-Dy**			
Dy1	2.940(12)	Dy2	2.696(10)
Dy3	2.929(13)	Dy4	2.895(13)
Dy5	2.741(11)	Dy6	2.862(13)
	+2	+3	+4
Mn1	3.338(17)	3.078(16)	3.020(15)
Mn2	3.416(18)	3.150(16)	3.091(16)
Mn3	3.357(18)	3.095(16)	3.037(16)

Mn4	3.350(17)	3.089(16)	3.031(15)
Mn5	3.423(19)	3.088(17)	2.909(17)
Mn6	3.450(21)	3.213(20)	2.930(19)
Mn7	3.511(21)	3.270(20)	3.069(19)
Mn8	3.486(26)	3.247(24)	3.034(23)
Mn9	3.455(21)	3.219(20)	3.144(19)
Mn10	3.455(21)	3.209(20)	3.134(19)
Mn11	3.454(22)	3.218(20)	3.016(20)
Mn12	3.446(19)	3.210(18)	2.978(17)
		Complex **2-Y**	
Y1	2.940(12)	Y2	2.696(10)
Y3	2.929(13)	Y4	2.895(13)
Y5	2.741(11)	Y6	2.862(13)
	+2	+3	+4
Mn1			
Mn2	3.338(17)	3.078(16)	3.020(15)
Mn3			
	3.416(18)	3.150(16)	3.091(16)
	3.357(18)	3.095(16)	3.037(16)
Mn4	3.350(17)	3.089(16)	3.031(15)
Mn5	3.423(19)	3.088(17)	2.909(17)
Mn6	3.450(21)	3.213(20)	2.930(19)
Mn7	3.511(21)	3.270(20)	3.069(19)
Mn8	3.486(26)	3.247(24)	3.034(23)
Mn9	3.455(21)	3.219(20)	3.144(19)
Mn10	3.455(21)	3.209(20)	3.134(19)
Mn11	3.454(22)	3.218(20)	3.016(20)
Mn12	3.446(19)	3.210(18)	2.978(17)

Table S2. Bond lengths [Å] and angles [°] for **1-Dy**, **2-Dy** and **2-Y**.

		1-Dy	
Dy(1)-O(19)	2.306(10)	Mn(1)-O(6)	1.968(8)
Dy(1)-O(14)#1	2.336(11)	Mn(1)-O(3)	2.100(2)
Dy(1)-O(8)	2.341(10)	Mn(1)-O(13)	2.152(10)
Dy(1)-O(17)	2.347(8)	Mn(2)-O(7)	1.888(9)
Dy(1)-O(5)	2.357(8)	Mn(2)-O(8)	1.916(9)
Dy(1)-O(4)	2.434(8)	Mn(2)-O(1)	1.918(8)
Dy(1)-O(2)	2.436(4)	Mn(2)-N(1)	1.969(12)
Dy(1)-O(11)	2.608(9)	Mn(2)-O(15)	2.227(8)
Dy(1)-O(1)	2.686(7)	Mn(2)-O(13)	2.367(8)
Dy(2)-O(1)	2.328(8)	Mn(3)-O(10)	1.868(9)
Dy(2)-O(5)	2.394(8)	Mn(3)-O(11)	1.878(9)
Dy(2)-O(4)	2.456(7)	Mn(3)-O(4)	1.916(8)
Dy(2)-O(16)	2.480(9)	Mn(3)-N(2)	1.967(12)
Mn(1)-O(1)	1.886(8)	Mn(3)-O(18)	2.178(10)
Mn(1)-O(2)	1.913(8)	Mn(3)-O(16)#2	2.444(8)
Mn(1)-O(5)#1	1.959(8)	O(5)#1-Mn(1)-O(6)	88.8(3)
O(19)-Dy(1)-O(14)#1	77.0(4)	O(1)-Mn(1)-O(3)	91.9(3)
O(19)-Dy(1)-O(8)	74.5(4)	O(2)-Mn(1)-O(3)	85.4(3)

O(14)#1-Dy(1)-O(8)	150.2(3)	O(5)#1-Mn(1)-O(3)	87.1(2)
O(19)-Dy(1)-O(17)	74.5(3)	O(6)-Mn(1)-O(3)	84.4(3)
O(14)#1-Dy(1)-O(17)	86.0(3)	O(1)-Mn(1)-O(13)	84.3(3)
O(8)-Dy(1)-O(17)	78.0(3)	O(2)-Mn(1)-O(13)	96.9(4)
O(19)-Dy(1)-O(5)	140.2(3)	O(5)#1-Mn(1)-O(13)	96.9(3)
O(14)#1-Dy(1)-O(5)	79.9(3)	O(6)-Mn(1)-O(13)	93.6(4)
O(8)-Dy(1)-O(5)	128.7(3)	O(3)-Mn(1)-O(13)	175.5(2)
O(17)-Dy(1)-O(5)	135.6(3)	O(7)-Mn(2)-O(8)	172.7(4)
O(19)-Dy(1)-O(4)	147.5(3)	O(7)-Mn(2)-O(1)	98.8(4)
O(14)#1-Dy(1)-O(4)	129.2(3)	O(8)-Mn(2)-O(1)	88.5(4)
O(8)-Dy(1)-O(4)	75.5(3)	O(7)-Mn(2)-N(1)	89.7(5)
O(17)-Dy(1)-O(4)	87.4(3)	O(8)-Mn(2)-N(1)	83.0(4)
O(5)-Dy(1)-O(4)	70.5(3)	O(1)-Mn(2)-N(1)	169.5(4)
O(19)-Dy(1)-O(2)	78.1(3)	O(7)-Mn(2)-O(15)	90.6(3)
O(14)#1-Dy(1)-O(2)	81.0(2)	O(8)-Mn(2)-O(15)	89.6(3)
O(8)-Dy(1)-O(2)	101.6(2)	O(1)-Mn(2)-O(15)	95.7(3)
O(17)-Dy(1)-O(2)	151.7(3)	N(1)-Mn(2)-O(15)	90.4(4)
O(5)-Dy(1)-O(2)	66.5(3)	O(7)-Mn(2)-O(13)	90.7(3)
O(4)-Dy(1)-O(2)	120.2(3)	O(8)-Mn(2)-O(13)	89.9(3)
O(19)-Dy(1)-O(11)	132.5(3)	O(1)-Mn(2)-O(13)	77.9(3)
O(14)#1-Dy(1)-O(11)	68.6(3)	N(1)-Mn(2)-O(13)	95.9(4)
O(8)-Dy(1)-O(11)	127.4(3)	O(15)-Mn(2)-O(13)	173.6(4)
O(17)-Dy(1)-O(11)	71.6(3)	O(10)-Mn(3)-O(11)	174.8(5)
O(5)-Dy(1)-O(11)	64.1(3)	O(10)-Mn(3)-O(4)	97.9(4)
O(4)-Dy(1)-O(11)	61.6(3)	O(11)-Mn(3)-O(4)	86.0(4)
O(2)-Dy(1)-O(11)	125.2(2)	O(10)-Mn(3)-N(2)	90.7(5)
O(19)-Dy(1)-O(1)	112.7(3)	O(11)-Mn(3)-N(2)	85.3(5)
O(14)#1-Dy(1)-O(1)	137.8(3)	O(4)-Mn(3)-N(2)	170.8(4)
O(8)-Dy(1)-O(1)	63.9(3)	O(10)-Mn(3)-O(18)	90.7(4)
O(17)-Dy(1)-O(1)	136.0(3)	O(11)-Mn(3)-O(18)	92.4(4)
O(5)-Dy(1)-O(1)	66.9(3)	O(4)-Mn(3)-O(18)	95.0(4)
O(4)-Dy(1)-O(1)	63.3(2)	N(2)-Mn(3)-O(18)	88.2(4)
O(2)-Dy(1)-O(1)	62.7(2)	O(10)-Mn(3)-O(16)#2	88.1(3)
O(11)-Dy(1)-O(1)	114.8(3)	O(11)-Mn(3)-O(16)#2	89.5(3)
O(1)#2-Dy(2)-O(1)	126.5(4)	O(4)-Mn(3)-O(16)#2	75.8(3)
O(1)#2-Dy(2)-O(5)	82.1(3)	N(2)-Mn(3)-O(16)#2	101.2(4)
O(1)-Dy(2)-O(5)	72.5(3)	O(18)-Mn(3)-O(16)#2	170.5(4)
O(1)#2-Dy(2)-O(5)#2	72.5(3)	Mn(1)-O(1)-Mn(2)	108.9(4)
O(1)-Dy(2)-O(5)#2	82.1(3)	Mn(1)-O(1)-Dy(2)	117.2(4)
O(5)-Dy(2)-O(5)#2	121.7(4)	Mn(2)-O(1)-Dy(2)	129.3(4)

O(1)#2-Dy(2)-O(4)	142.3(3)	Mn(1)-O(1)-Dy(1)	99.1(3)
O(1)-Dy(2)-O(4)	68.5(3)	Mn(2)-O(1)-Dy(1)	97.5(3)
O(5)-Dy(2)-O(4)	69.6(3)	Dy(2)-O(1)-Dy(1)	95.0(3)
O(5)#2-Dy(2)-O(4)	143.9(3)	Mn(1)#1-O(2)-Mn(1)	100.3(5)
O(1)#2-Dy(2)-O(4)#2	68.5(3)	Mn(1)#1-O(2)-Dy(1)#1	107.28(10)
O(1)-Dy(2)-O(4)#2	142.3(3)	Mn(1)-O(2)-Dy(1)#1	99.45(9)
O(5)-Dy(2)-O(4)#2	143.9(3)	Mn(1)#1-O(2)-Dy(1)	99.45(9)
O(5)#2-Dy(2)-O(4)#2	69.6(3)	Mn(1)-O(2)-Dy(1)	107.28(10)
O(4)-Dy(2)-O(4)#2	123.8(4)	Dy(1)#1-O(2)-Dy(1)	137.8(5)
O(1)#2-Dy(2)-O(16)	132.9(3)	Mn(1)#1-O(3)-Mn(1)#2	91.45(11)
O(1)-Dy(2)-O(16)	84.5(3)	Mn(1)#1-O(3)-Mn(1)	88.79(11)
O(5)-Dy(2)-O(16)	145.0(3)	Mn(1)#2-O(3)-Mn(1)	174.73(9)
O(5)#2-Dy(2)-O(16)	79.2(3)	Mn(1)#1-O(3)-Mn(1)#3	174.73(9)
O(4)-Dy(2)-O(16)	77.7(3)	Mn(1)#2-O(3)-Mn(1)#3	88.79(11)
O(4)#2-Dy(2)-O(16)	66.6(3)	Mn(1)-O(3)-Mn(1)#3	91.45(11)
O(1)#2-Dy(2)-O(16)#2	84.5(3)	Mn(3)-O(4)-Dy(1)	104.9(3)
O(1)-Dy(2)-O(16)#2	132.9(3)	Mn(3)-O(4)-Dy(2)	117.8(4)
O(5)-Dy(2)-O(16)#2	79.2(3)	Dy(1)-O(4)-Dy(2)	98.5(3)
O(5)#2-Dy(2)-O(16)#2	145.0(3)	Mn(1)#1-O(5)-Dy(1)	100.8(3)
O(4)-Dy(2)-O(16)#2	66.6(3)	Mn(1)#1-O(5)-Dy(2)	119.3(3)
O(4)#2-Dy(2)-O(16)#2	77.7(3)	Dy(1)-O(5)-Dy(2)	102.5(3)
O(16)-Dy(2)-O(16)#2	99.2(4)	Mn(1)#3-O(6)-Mn(1)	99.7(5)
O(1)-Mn(1)-O(2)	89.4(2)	Mn(2)-O(8)-Dy(1)	110.1(4)
O(1)-Mn(1)-O(5)#1	174.8(4)	Mn(3)-O(11)-Dy(1)	99.8(4)
O(2)-Mn(1)-O(5)#1	85.5(3)	Mn(1)-O(13)-Mn(2)	86.3(3)
O(1)-Mn(1)-O(6)	96.2(2)	Mn(3)#2-O(16)-Dy(2)	99.3(3)
O(2)-Mn(1)-O(6)	168.6(4)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+9/4,y,-z+1/4 #2 -x+9/4,-y+5/4,z #3 x,-y+5/4,-z+1/4

2-Dy

Dy(1)-O(44)	2.288(4)	Mn(1)-O(12)	1.881(4)
Dy(1)-O(69)	2.325(4)	Mn(1)-O(18)	1.932(4)
Dy(1)-O(21)	2.345(4)	Mn(1)-O(5)	1.963(4)
Dy(1)-O(4)	2.388(4)	Mn(1)-O(1)	1.976(4)
Dy(1)-O(45)	2.425(5)	Mn(1)-O(9)	2.183(4)
Dy(1)-O(10)	2.452(4)	Mn(1)-O(4)	2.257(4)
Dy(1)-O(5)	2.479(4)	Mn(2)-O(2)	1.882(4)
Dy(1)-O(27)	2.497(4)	Mn(2)-O(4)	1.911(4)
Dy(1)-O(2)	2.691(4)	Mn(2)-O(6)	1.936(4)

Dy(2)-O(7)	2.348(4)	Mn(2)-O(13)	1.949(4)
Dy(2)-O(5)	2.350(4)	Mn(2)-O(54)	2.201(4)
Dy(2)-O(3)	2.394(4)	Mn(2)-O(1)	2.291(4)
Dy(2)-O(2)	2.402(4)	Mn(3)-O(3)	1.894(4)
Dy(2)-O(10)	2.440(4)	Mn(3)-O(8)	1.917(4)
Dy(2)-O(11)	2.464(4)	Mn(3)-O(9)	1.938(5)
Dy(2)-O(58)	2.496(4)	Mn(3)-O(15)	1.954(4)
Dy(2)-O(62)	2.511(4)	Mn(3)-O(56)	2.207(5)
Dy(2)-O(1)	2.780(4)	Mn(3)-O(1)	2.277(4)
Dy(3)-O(47)	2.314(5)	Mn(4)-O(14)	1.875(4)
Dy(3)-O(61)	2.321(5)	Mn(4)-O(19)	1.921(5)
Dy(3)-O(24)	2.362(5)	Mn(4)-O(7)	1.944(4)
Dy(3)-O(8)	2.364(4)	Mn(4)-O(1)	1.996(4)
Dy(3)-O(48)	2.401(5)	Mn(4)-O(6)	2.190(4)
Dy(3)-O(11)	2.444(4)	Mn(4)-O(8)	2.250(4)
Dy(3)-O(7)	2.482(4)	Mn(5)-O(21)	1.894(4)
Dy(3)-O(30)	2.506(5)	Mn(5)-O(2)	1.908(4)
Dy(3)-O(3)	2.697(5)	Mn(5)-O(20)	1.931(4)
Dy(4)-O(67)	2.279(5)	Mn(5)-N(1)	1.984(5)
Dy(4)-O(33)	2.330(4)	Mn(5)-O(63)	2.229(4)
Dy(4)-O(55)	2.345(5)	Mn(5)-O(54)	2.336(4)
Dy(4)-O(13)	2.389(4)	Mn(6)-O(24)	1.887(5)
Dy(4)-O(16)	2.399(4)	Mn(6)-O(3)	1.896(4)
Dy(4)-O(70)	2.401(5)	Mn(6)-O(23)	1.909(5)
Dy(4)-O(6)	2.434(4)	Mn(6)-N(2)	1.984(6)
Dy(4)-O(39)	2.469(5)	Mn(6)-O(59)	2.221(4)
Dy(5)-O(12)	2.248(4)	Mn(6)-O(56)	2.330(4)
Dy(5)-O(14)	2.256(4)	Mn(7)-O(27)	1.872(4)
Dy(5)-O(52)	2.443(5)	Mn(7)-O(26)	1.891(4)
Dy(5)-O(16)	2.453(4)	Mn(7)-O(10)	1.904(4)
Dy(5)-O(17)	2.454(5)	Mn(7)-N(3)	1.986(6)
Dy(5)-O(50)	2.456(4)	Mn(7)-O(68)	2.177(5)
Dy(5)-O(15)	2.466(4)	Mn(7)-O(58)	2.511(4)
Dy(5)-O(13)	2.484(4)	Mn(8)-O(29)	1.876(5)
Dy(6)-O(65)	2.309(5)	Mn(8)-O(30)	1.887(5)
Dy(6)-O(36)	2.319(5)	Mn(8)-O(11)	1.915(5)
Dy(6)-O(57)	2.342(5)	Mn(8)-N(4)	1.978(6)
Dy(6)-O(15)	2.377(5)	Mn(8)-O(60)	2.188(5)
Dy(6)-O(71)	2.399(5)	Mn(8)-O(62)	2.514(4)
Dy(6)-O(17)	2.408(4)	Mn(9)-O(14)	1.900(4)

Dy(6)-O(9)	2.445(4)	Mn(9)-O(33)	1.906(5)
Dy(6)-O(42)	2.470(5)	Mn(9)-O(32)	1.946(5)
Mn(10)-O(36)	1.912(4)	Mn(9)-N(5)	1.975(6)
Mn(10)-O(35)	1.944(5)	Mn(9)-O(19)	2.222(4)
Mn(10)-N(6)	1.981(6)	Mn(9)-O(51)	2.244(5)
Mn(10)-O(18)	2.194(4)	Mn(10)-O(12)	1.892(4)
Mn(10)-O(53)	2.270(5)	Mn(12)-O(42)	1.883(5)
Mn(11)-O(39)	1.871(4)	Mn(12)-O(41)	1.883(5)
Mn(11)-O(38)	1.885(5)	Mn(12)-O(17)	1.937(4)
Mn(11)-O(16)	1.941(4)	Mn(12)-N(8)	1.973(6)
Mn(11)-N(7)	1.972(6)	Mn(12)-O(64)	2.192(6)
Mn(11)-O(66)	2.188(5)	Mn(12)-O(50)	2.442(5)
Mn(11)-O(52)	2.509(5)		
O(44)-Dy(1)-O(69)	84.77(16)	O(3)-Dy(2)-O(58)	84.40(14)
O(44)-Dy(1)-O(21)	143.96(14)	O(2)-Dy(2)-O(58)	130.26(14)
O(69)-Dy(1)-O(21)	75.34(15)	O(10)-Dy(2)-O(58)	65.82(14)
O(44)-Dy(1)-O(4)	79.14(14)	O(11)-Dy(2)-O(58)	75.04(15)
O(69)-Dy(1)-O(4)	146.51(15)	O(7)-Dy(2)-O(62)	75.31(14)
O(21)-Dy(1)-O(4)	101.35(14)	O(5)-Dy(2)-O(62)	145.61(13)
O(44)-Dy(1)-O(45)	72.24(16)	O(3)-Dy(2)-O(62)	129.81(14)
O(69)-Dy(1)-O(45)	73.37(16)	O(2)-Dy(2)-O(62)	83.78(13)
O(21)-Dy(1)-O(45)	73.38(15)	O(10)-Dy(2)-O(62)	74.56(14)
O(4)-Dy(1)-O(45)	73.81(15)	O(11)-Dy(2)-O(62)	65.68(14)
O(44)-Dy(1)-O(10)	136.67(15)	O(58)-Dy(2)-O(62)	98.41(15)
O(69)-Dy(1)-O(10)	92.02(14)	O(7)-Dy(2)-O(1)	63.75(13)
O(21)-Dy(1)-O(10)	74.71(14)	O(5)-Dy(2)-O(1)	63.61(13)
O(4)-Dy(1)-O(10)	119.69(13)	O(3)-Dy(2)-O(1)	65.66(12)
O(45)-Dy(1)-O(10)	147.34(15)	O(2)-Dy(2)-O(1)	65.49(12)
O(44)-Dy(1)-O(5)	84.92(14)	O(10)-Dy(2)-O(1)	121.37(12)
O(69)-Dy(1)-O(5)	139.70(15)	O(11)-Dy(2)-O(1)	120.61(13)
O(21)-Dy(1)-O(5)	129.18(14)	O(58)-Dy(2)-O(1)	131.41(14)
O(4)-Dy(1)-O(5)	67.98(13)	O(62)-Dy(2)-O(1)	130.17(14)
O(45)-Dy(1)-O(5)	138.45(14)	O(47)-Dy(3)-O(61)	83.99(18)
O(10)-Dy(1)-O(5)	70.04(13)	O(47)-Dy(3)-O(24)	143.14(16)
O(44)-Dy(1)-O(27)	74.95(15)	O(61)-Dy(3)-O(24)	75.69(19)
O(69)-Dy(1)-O(27)	73.10(15)	O(47)-Dy(3)-O(8)	79.67(16)
O(21)-Dy(1)-O(27)	125.09(15)	O(61)-Dy(3)-O(8)	147.77(15)
O(4)-Dy(1)-O(27)	128.98(14)	O(24)-Dy(3)-O(8)	101.71(16)
O(45)-Dy(1)-O(27)	134.53(16)	O(47)-Dy(3)-O(48)	72.52(18)
O(10)-Dy(1)-O(27)	62.91(14)	O(61)-Dy(3)-O(48)	74.66(17)

O(5)-Dy(1)-O(27)	66.60(14)	O(24)-Dy(3)-O(48)	72.59(18)
O(44)-Dy(1)-O(2)	138.81(13)	O(8)-Dy(3)-O(48)	74.00(15)
O(69)-Dy(1)-O(2)	135.85(14)	O(47)-Dy(3)-O(11)	137.06(16)
O(21)-Dy(1)-O(2)	63.82(13)	O(61)-Dy(3)-O(11)	91.18(16)
O(4)-Dy(1)-O(2)	62.53(13)	O(24)-Dy(3)-O(11)	74.60(16)
O(45)-Dy(1)-O(2)	108.13(14)	O(8)-Dy(3)-O(11)	119.51(14)
O(10)-Dy(1)-O(2)	62.51(12)	O(48)-Dy(3)-O(11)	146.55(17)
O(5)-Dy(1)-O(2)	67.80(13)	O(47)-Dy(3)-O(7)	87.09(15)
O(27)-Dy(1)-O(2)	117.30(13)	O(61)-Dy(3)-O(7)	139.17(16)
O(7)-Dy(2)-O(5)	127.35(14)	O(24)-Dy(3)-O(7)	127.97(15)
O(7)-Dy(2)-O(3)	74.80(15)	O(8)-Dy(3)-O(7)	67.64(14)
O(5)-Dy(2)-O(3)	84.05(14)	O(48)-Dy(3)-O(7)	139.17(15)
O(7)-Dy(2)-O(2)	83.87(14)	O(11)-Dy(3)-O(7)	69.22(14)
O(5)-Dy(2)-O(2)	74.88(14)	O(47)-Dy(3)-O(30)	74.26(16)
O(3)-Dy(2)-O(2)	131.15(13)	O(61)-Dy(3)-O(30)	73.53(17)
O(7)-Dy(2)-O(10)	139.88(14)	O(24)-Dy(3)-O(30)	126.50(16)
O(5)-Dy(2)-O(10)	72.41(13)	O(8)-Dy(3)-O(30)	126.97(15)
O(3)-Dy(2)-O(10)	145.30(15)	O(48)-Dy(3)-O(30)	135.73(17)
O(2)-Dy(2)-O(10)	67.11(13)	O(11)-Dy(3)-O(30)	63.54(16)
O(7)-Dy(2)-O(11)	71.07(14)	O(7)-Dy(3)-O(30)	65.70(14)
O(5)-Dy(2)-O(11)	140.83(15)	O(47)-Dy(3)-O(3)	140.19(14)
O(3)-Dy(2)-O(11)	66.89(14)	O(61)-Dy(3)-O(3)	135.22(17)
O(2)-Dy(2)-O(11)	144.19(15)	O(24)-Dy(3)-O(3)	63.09(14)
O(10)-Dy(2)-O(11)	118.01(14)	O(8)-Dy(3)-O(3)	62.79(13)
O(7)-Dy(2)-O(58)	145.05(14)	O(48)-Dy(3)-O(3)	106.81(16)
O(5)-Dy(2)-O(58)	76.55(14)	O(11)-Dy(3)-O(3)	62.56(13)
O(55)-Dy(4)-O(6)	81.14(14)	O(7)-Dy(3)-O(3)	67.43(14)
O(13)-Dy(4)-O(6)	65.75(14)	O(30)-Dy(3)-O(3)	117.44(13)
O(16)-Dy(4)-O(6)	119.38(14)	O(67)-Dy(4)-O(33)	79.63(17)
O(70)-Dy(4)-O(6)	75.20(16)	O(67)-Dy(4)-O(55)	93.13(17)
O(67)-Dy(4)-O(39)	73.94(17)	O(33)-Dy(4)-O(55)	147.38(17)
O(33)-Dy(4)-O(39)	134.54(15)	O(67)-Dy(4)-O(13)	142.93(17)
O(55)-Dy(4)-O(39)	71.21(15)	O(33)-Dy(4)-O(13)	123.70(15)
O(13)-Dy(4)-O(39)	69.40(14)	O(55)-Dy(4)-O(13)	80.38(15)
O(16)-Dy(4)-O(39)	64.02(15)	O(67)-Dy(4)-O(16)	86.01(17)
O(70)-Dy(4)-O(39)	129.60(17)	O(33)-Dy(4)-O(16)	78.02(16)
O(6)-Dy(4)-O(39)	130.28(14)	O(55)-Dy(4)-O(16)	133.60(16)
O(12)-Dy(5)-O(14)	118.71(14)	O(13)-Dy(4)-O(16)	73.36(14)
O(12)-Dy(5)-O(52)	85.85(15)	O(67)-Dy(4)-O(70)	74.69(18)
O(14)-Dy(5)-O(52)	136.15(16)	O(33)-Dy(4)-O(70)	75.19(17)

O(12)-Dy(5)-O(16)	142.05(15)	O(55)-Dy(4)-O(70)	72.22(17)
O(14)-Dy(5)-O(16)	71.26(15)	O(13)-Dy(4)-O(70)	135.06(16)
O(52)-Dy(5)-O(16)	68.14(16)	O(16)-Dy(4)-O(70)	149.29(16)
O(12)-Dy(5)-O(17)	72.27(14)	O(67)-Dy(4)-O(6)	149.67(17)
O(14)-Dy(5)-O(17)	142.90(15)	O(33)-Dy(4)-O(6)	89.26(15)
O(52)-Dy(5)-O(17)	76.46(16)	O(17)-Dy(5)-O(13)	141.22(15)
O(16)-Dy(5)-O(17)	123.80(14)	O(50)-Dy(5)-O(13)	146.52(15)
O(12)-Dy(5)-O(50)	136.19(15)	O(15)-Dy(5)-O(13)	123.14(13)
O(14)-Dy(5)-O(50)	86.96(15)	O(65)-Dy(6)-O(36)	79.50(17)
O(52)-Dy(5)-O(50)	99.50(15)	O(65)-Dy(6)-O(57)	92.35(18)
O(16)-Dy(5)-O(50)	77.27(15)	O(36)-Dy(6)-O(57)	147.24(18)
O(17)-Dy(5)-O(50)	67.03(15)	O(65)-Dy(6)-O(15)	143.62(16)
O(12)-Dy(5)-O(15)	74.31(15)	O(36)-Dy(6)-O(15)	122.56(15)
O(14)-Dy(5)-O(15)	78.58(15)	O(57)-Dy(6)-O(15)	82.07(17)
O(52)-Dy(5)-O(15)	145.25(16)	O(65)-Dy(6)-O(71)	74.14(18)
O(16)-Dy(5)-O(15)	141.28(15)	O(36)-Dy(6)-O(71)	74.44(18)
O(17)-Dy(5)-O(15)	70.49(14)	O(57)-Dy(6)-O(71)	72.82(19)
O(50)-Dy(5)-O(15)	77.44(14)	O(15)-Dy(6)-O(71)	136.05(16)
O(12)-Dy(5)-O(13)	77.26(15)	O(65)-Dy(6)-O(17)	86.68(17)
O(14)-Dy(5)-O(13)	73.65(14)	O(36)-Dy(6)-O(17)	77.10(16)
O(52)-Dy(5)-O(13)	77.99(14)	O(57)-Dy(6)-O(17)	134.53(16)
O(16)-Dy(5)-O(13)	70.80(14)	O(15)-Dy(6)-O(17)	72.80(15)
O(12)-Mn(1)-O(18)	86.06(18)	O(71)-Dy(6)-O(17)	148.02(18)
O(12)-Mn(1)-O(5)	175.56(18)	O(65)-Dy(6)-O(9)	149.54(16)
O(18)-Mn(1)-O(5)	91.35(18)	O(36)-Dy(6)-O(9)	89.44(14)
O(12)-Mn(1)-O(1)	94.87(18)	O(57)-Dy(6)-O(9)	81.71(15)
O(18)-Mn(1)-O(1)	178.65(18)	O(15)-Dy(6)-O(9)	65.39(14)
O(5)-Mn(1)-O(1)	87.66(17)	O(71)-Dy(6)-O(9)	75.57(16)
O(12)-Mn(1)-O(9)	85.81(17)	O(17)-Dy(6)-O(9)	118.60(14)
O(18)-Mn(1)-O(9)	92.11(18)	O(65)-Dy(6)-O(42)	74.39(17)
O(5)-Mn(1)-O(9)	97.89(16)	O(36)-Dy(6)-O(42)	134.09(16)
O(1)-Mn(1)-O(9)	88.94(17)	O(57)-Dy(6)-O(42)	71.55(16)
O(12)-Mn(1)-O(4)	96.40(17)	O(15)-Dy(6)-O(42)	69.73(15)
O(18)-Mn(1)-O(4)	90.59(17)	O(71)-Dy(6)-O(42)	130.66(17)
O(5)-Mn(1)-O(4)	80.01(15)	O(17)-Dy(6)-O(42)	64.45(15)
O(1)-Mn(1)-O(4)	88.33(16)	O(9)-Dy(6)-O(42)	130.13(15)
O(9)-Mn(1)-O(4)	176.62(16)	O(8)-Mn(3)-O(1)	88.60(17)
O(2)-Mn(2)-O(4)	88.60(17)	O(9)-Mn(3)-O(1)	87.20(17)
O(2)-Mn(2)-O(6)	94.57(18)	O(15)-Mn(3)-O(1)	89.43(16)
O(4)-Mn(2)-O(6)	175.16(18)	O(56)-Mn(3)-O(1)	166.65(16)

O(2)-Mn(2)-O(13)	173.71(17)	O(14)-Mn(4)-O(19)	87.58(19)
O(4)-Mn(2)-O(13)	91.70(18)	O(14)-Mn(4)-O(7)	175.57(18)
O(6)-Mn(2)-O(13)	84.75(18)	O(19)-Mn(4)-O(7)	90.30(19)
O(2)-Mn(2)-O(54)	84.02(16)	O(14)-Mn(4)-O(1)	94.23(18)
O(4)-Mn(2)-O(54)	95.78(17)	O(19)-Mn(4)-O(1)	177.91(18)
O(6)-Mn(2)-O(54)	88.21(17)	O(7)-Mn(4)-O(1)	87.82(18)
O(13)-Mn(2)-O(54)	102.20(16)	O(14)-Mn(4)-O(6)	85.39(17)
O(2)-Mn(2)-O(1)	84.46(15)	O(19)-Mn(4)-O(6)	92.13(18)
O(4)-Mn(2)-O(1)	88.97(16)	O(7)-Mn(4)-O(6)	98.59(16)
O(6)-Mn(2)-O(1)	87.69(16)	O(1)-Mn(4)-O(6)	89.07(16)
O(13)-Mn(2)-O(1)	89.26(16)	O(14)-Mn(4)-O(8)	96.39(17)
O(54)-Mn(2)-O(1)	167.42(16)	O(19)-Mn(4)-O(8)	91.30(18)
O(3)-Mn(3)-O(8)	88.17(19)	O(7)-Mn(4)-O(8)	79.76(16)
O(3)-Mn(3)-O(9)	95.48(19)	O(1)-Mn(4)-O(8)	87.46(16)
O(8)-Mn(3)-O(9)	174.15(19)	O(6)-Mn(4)-O(8)	176.21(16)
O(3)-Mn(3)-O(15)	174.12(17)	O(21)-Mn(5)-O(2)	89.59(18)
O(8)-Mn(3)-O(15)	91.87(19)	O(21)-Mn(5)-O(20)	173.12(18)
O(9)-Mn(3)-O(15)	84.03(19)	O(2)-Mn(5)-O(20)	97.09(17)
O(3)-Mn(3)-O(56)	83.63(17)	O(21)-Mn(5)-N(1)	83.3(2)
O(8)-Mn(3)-O(56)	97.46(19)	O(2)-Mn(5)-N(1)	170.0(2)
O(9)-Mn(3)-O(56)	87.51(19)	O(20)-Mn(5)-N(1)	89.9(2)
O(15)-Mn(3)-O(56)	102.19(17)	O(21)-Mn(5)-O(63)	90.14(17)
O(3)-Mn(3)-O(1)	84.69(16)	O(2)-Mn(5)-O(63)	96.23(16)
O(3)-Mn(6)-O(23)	97.12(19)	O(20)-Mn(5)-O(63)	90.79(18)
O(24)-Mn(6)-N(2)	83.4(2)	N(1)-Mn(5)-O(63)	90.82(18)
O(3)-Mn(6)-N(2)	170.7(2)	O(21)-Mn(5)-O(54)	89.58(17)
O(23)-Mn(6)-N(2)	89.9(2)	O(2)-Mn(5)-O(54)	79.83(16)
O(24)-Mn(6)-O(59)	89.3(2)	O(20)-Mn(5)-O(54)	89.96(17)
O(3)-Mn(6)-O(59)	95.90(17)	N(1)-Mn(5)-O(54)	93.07(18)
O(23)-Mn(6)-O(59)	91.1(2)	O(63)-Mn(5)-O(54)	176.05(16)
N(2)-Mn(6)-O(59)	90.0(2)	O(24)-Mn(6)-O(3)	89.5(2)
O(24)-Mn(6)-O(56)	90.01(19)	O(24)-Mn(6)-O(23)	173.3(2)
O(3)-Mn(6)-O(56)	80.26(16)	O(11)-Mn(8)-O(60)	94.96(19)
O(23)-Mn(6)-O(56)	90.06(19)	N(4)-Mn(8)-O(60)	87.8(2)
N(2)-Mn(6)-O(56)	93.7(2)	O(29)-Mn(8)-O(62)	89.16(18)
O(59)-Mn(6)-O(56)	176.10(17)	O(30)-Mn(8)-O(62)	87.72(18)
O(27)-Mn(7)-O(26)	174.4(2)	O(11)-Mn(8)-O(62)	73.67(16)
O(27)-Mn(7)-O(10)	86.31(18)	N(4)-Mn(8)-O(62)	103.7(2)
O(26)-Mn(7)-O(10)	97.22(19)	O(60)-Mn(8)-O(62)	168.48(18)
O(27)-Mn(7)-N(3)	84.3(2)	O(14)-Mn(9)-O(33)	89.32(19)

O(26)-Mn(7)-N(3)	91.9(2)	O(14)-Mn(9)-O(32)	97.5(2)
O(10)-Mn(7)-N(3)	169.9(2)	O(33)-Mn(9)-O(32)	173.1(2)
O(27)-Mn(7)-O(68)	92.6(2)	O(14)-Mn(9)-N(5)	172.2(2)
O(26)-Mn(7)-O(68)	91.4(2)	O(33)-Mn(9)-N(5)	84.0(2)
O(10)-Mn(7)-O(68)	96.37(18)	O(32)-Mn(9)-N(5)	89.2(2)
N(3)-Mn(7)-O(68)	87.7(2)	O(14)-Mn(9)-O(19)	78.76(17)
O(27)-Mn(7)-O(58)	87.15(18)	O(33)-Mn(9)-O(19)	90.28(18)
O(26)-Mn(7)-O(58)	89.69(18)	O(32)-Mn(9)-O(19)	91.87(18)
O(10)-Mn(7)-O(58)	73.38(16)	N(5)-Mn(9)-O(19)	97.1(2)
N(3)-Mn(7)-O(58)	102.5(2)	O(14)-Mn(9)-O(51)	92.00(17)
O(68)-Mn(7)-O(58)	169.75(17)	O(33)-Mn(9)-O(51)	91.63(19)
O(29)-Mn(8)-O(30)	173.8(2)	O(32)-Mn(9)-O(51)	87.31(19)
O(29)-Mn(8)-O(11)	97.7(2)	N(5)-Mn(9)-O(51)	92.3(2)
O(30)-Mn(8)-O(11)	86.6(2)	O(19)-Mn(9)-O(51)	170.55(18)
O(29)-Mn(8)-N(4)	91.2(2)	O(12)-Mn(10)-O(36)	89.75(19)
O(30)-Mn(8)-N(4)	84.4(2)	O(12)-Mn(10)-O(35)	97.25(19)
O(11)-Mn(8)-N(4)	170.7(2)	O(36)-Mn(10)-O(35)	172.6(2)
O(29)-Mn(8)-O(60)	90.6(2)	O(12)-Mn(10)-N(6)	172.5(2)
O(30)-Mn(8)-O(60)	93.5(2)	O(36)-Mn(10)-N(6)	83.5(2)
O(18)-Mn(10)-O(53)	170.84(18)	O(35)-Mn(10)-N(6)	89.7(2)
O(39)-Mn(11)-O(38)	174.3(2)	O(12)-Mn(10)-O(18)	78.74(17)
O(39)-Mn(11)-O(16)	85.21(19)	O(36)-Mn(10)-O(18)	92.08(18)
O(38)-Mn(11)-O(16)	98.8(2)	O(35)-Mn(10)-O(18)	91.69(17)
O(39)-Mn(11)-N(7)	84.5(2)	N(6)-Mn(10)-O(18)	98.4(2)
O(38)-Mn(11)-N(7)	91.2(2)	O(12)-Mn(10)-O(53)	92.18(17)
O(16)-Mn(11)-N(7)	169.0(2)	O(36)-Mn(10)-O(53)	89.03(18)
O(39)-Mn(11)-O(66)	92.9(2)	O(35)-Mn(10)-O(53)	88.25(18)
O(38)-Mn(11)-O(66)	90.7(2)	N(6)-Mn(10)-O(53)	90.8(2)
O(16)-Mn(11)-O(66)	96.1(2)	Mn(3)-O(1)-Mn(2)	175.1(2)
N(7)-Mn(11)-O(66)	88.3(2)	Mn(1)-O(1)-Dy(2)	96.19(15)
O(39)-Mn(11)-O(52)	88.33(18)	Mn(4)-O(1)-Dy(2)	95.37(15)
O(38)-Mn(11)-O(52)	88.78(19)	Mn(3)-O(1)-Dy(2)	92.47(13)
O(16)-Mn(11)-O(52)	74.90(18)	Mn(2)-O(1)-Dy(2)	92.39(13)
N(7)-Mn(11)-O(52)	101.0(2)	Mn(2)-O(2)-Mn(5)	108.37(19)
O(66)-Mn(11)-O(52)	170.75(18)	Mn(2)-O(2)-Dy(2)	117.66(17)
O(42)-Mn(12)-O(41)	174.9(2)	Mn(5)-O(2)-Dy(2)	130.51(19)
O(42)-Mn(12)-O(17)	85.85(19)	Mn(2)-O(2)-Dy(1)	98.51(16)
O(41)-Mn(12)-O(17)	98.8(2)	Mn(5)-O(2)-Dy(1)	96.76(15)
O(42)-Mn(12)-N(8)	84.3(2)	Dy(2)-O(2)-Dy(1)	93.66(13)
O(41)-Mn(12)-N(8)	91.0(2)	Mn(3)-O(3)-Mn(6)	108.5(2)

O(17)-Mn(12)-N(8)	169.9(2)	Mn(3)-O(3)-Dy(2)	117.17(18)
O(42)-Mn(12)-O(64)	91.3(2)	Mn(6)-O(3)-Dy(2)	130.52(19)
O(41)-Mn(12)-O(64)	90.4(2)	Mn(3)-O(3)-Dy(3)	97.87(17)
O(17)-Mn(12)-O(64)	95.6(2)	Mn(6)-O(3)-Dy(3)	97.39(16)
N(8)-Mn(12)-O(64)	86.7(2)	Dy(2)-O(3)-Dy(3)	94.42(14)
O(42)-Mn(12)-O(50)	89.51(19)	Mn(2)-O(4)-Mn(1)	92.24(16)
O(41)-Mn(12)-O(50)	89.6(2)	Mn(2)-O(4)-Dy(1)	108.71(17)
O(17)-Mn(12)-O(50)	75.54(17)	Mn(1)-O(4)-Dy(1)	101.45(15)
N(8)-Mn(12)-O(50)	102.3(2)	Mn(1)-O(5)-Dy(2)	111.93(19)
O(64)-Mn(12)-O(50)	171.02(17)	Mn(1)-O(5)-Dy(1)	107.59(17)
Mn(1)-O(1)-Mn(4)	168.4(2)	Dy(2)-O(5)-Dy(1)	100.73(14)
Mn(1)-O(1)-Mn(3)	90.01(16)	Mn(2)-O(6)-Mn(4)	93.93(18)
Mn(4)-O(1)-Mn(3)	90.15(15)	Mn(2)-O(6)-Dy(4)	100.30(18)
Mn(1)-O(1)-Mn(2)	89.55(15)	Mn(4)-O(6)-Dy(4)	110.23(16)
Mn(4)-O(1)-Mn(2)	89.32(16)	Mn(4)-O(7)-Dy(2)	112.3(2)
Mn(7)-O(10)-Dy(1)	101.06(17)	Mn(4)-O(7)-Dy(3)	107.41(17)
Dy(2)-O(10)-Dy(1)	98.97(14)	Dy(2)-O(7)-Dy(3)	101.51(16)
Mn(8)-O(11)-Dy(3)	101.10(19)	Dy(6)-O(17)-Dy(5)	101.09(15)
Mn(8)-O(11)-Dy(2)	121.2(2)	Mn(3)-O(8)-Mn(4)	93.01(17)
Dy(3)-O(11)-Dy(2)	99.35(15)	Mn(3)-O(8)-Dy(3)	109.28(19)
Mn(1)-O(12)-Mn(10)	102.8(2)	Mn(4)-O(8)-Dy(3)	101.80(16)
Mn(1)-O(12)-Dy(5)	121.4(2)	Mn(3)-O(9)-Mn(1)	93.85(18)
Mn(10)-O(12)-Dy(5)	133.7(2)	Mn(3)-O(9)-Dy(6)	100.12(18)
Mn(2)-O(13)-Dy(4)	101.51(18)	Mn(1)-O(9)-Dy(6)	111.29(17)
Mn(2)-O(13)-Dy(5)	121.56(19)	Mn(7)-O(10)-Dy(2)	121.62(19)
Dy(4)-O(13)-Dy(5)	100.62(15)	Mn(5)-O(21)-Dy(1)	109.79(18)
Mn(4)-O(14)-Mn(9)	102.0(2)	Mn(6)-O(24)-Dy(3)	109.99(19)
Mn(4)-O(14)-Dy(5)	122.0(2)	Mn(7)-O(27)-Dy(1)	100.46(19)
Mn(9)-O(14)-Dy(5)	133.0(2)	Mn(8)-O(30)-Dy(3)	99.8(2)
Mn(3)-O(15)-Dy(6)	102.04(19)	Mn(9)-O(33)-Dy(4)	116.3(2)
Mn(3)-O(15)-Dy(5)	121.47(18)	Mn(10)-O(36)-Dy(6)	117.3(2)
Dy(6)-O(15)-Dy(5)	101.65(16)	Mn(11)-O(39)-Dy(4)	101.6(2)
Mn(11)-O(16)-Dy(4)	102.04(19)	Mn(12)-O(42)-Dy(6)	101.4(2)
Mn(11)-O(16)-Dy(5)	117.7(2)	Mn(12)-O(50)-Dy(5)	100.19(17)
Dy(4)-O(16)-Dy(5)	101.24(15)	Mn(2)-O(54)-Mn(5)	85.21(14)
Mn(12)-O(17)-Dy(6)	101.98(19)	Mn(3)-O(56)-Mn(6)	85.30(15)
Mn(12)-O(17)-Dy(5)	117.2(2)	Dy(2)-O(58)-Mn(7)	98.79(15)
Mn(1)-O(18)-Mn(10)	91.02(17)	Dy(2)-O(62)-Mn(8)	99.10(15)
Mn(4)-O(19)-Mn(9)	89.84(18)		

2-Y

Y(1)-O(44)	2.263(8)	Mn(2)-O(54)	2.193(6)
Y(1)-O(69)	2.324(7)	Mn(2)-O(1)	2.280(6)
Y(1)-O(21)	2.333(6)	Mn(3)-O(3)	1.886(6)
Y(1)-O(4)	2.374(6)	Mn(3)-O(8)	1.899(8)
Y(1)-O(45)	2.385(8)	Mn(3)-O(15)	1.952(6)
Y(1)-O(10)	2.417(7)	Mn(3)-O(9)	1.956(7)
Y(1)-O(5)	2.466(7)	Mn(3)-O(56)	2.202(7)
Y(1)-O(27)	2.491(6)	Mn(3)-O(1)	2.290(6)
Y(1)-O(2)	2.702(7)	Mn(4)-O(14)	1.850(6)
Y(2)-O(5)	2.326(8)	Mn(4)-O(19)	1.921(7)
Y(2)-O(7)	2.344(7)	Mn(4)-O(7)	1.968(6)
Y(2)-O(2)	2.389(6)	Mn(4)-O(1)	1.988(7)
Y(2)-O(3)	2.409(6)	Mn(4)-O(6)	2.213(6)
Y(2)-O(11)	2.446(8)	Mn(4)-O(8)	2.260(6)
Y(2)-O(10)	2.459(6)	Mn(5)-O(21)	1.896(7)
Y(2)-O(58)	2.474(6)	Mn(5)-O(2)	1.899(5)
Y(2)-O(62)	2.487(7)	Mn(5)-O(20)	1.925(7)
Y(2)-O(1)	2.766(5)	Mn(5)-N(1)	1.991(8)
Y(3)-O(61)	2.286(9)	Mn(5)-O(63)	2.235(7)
Y(3)-O(47)	2.319(9)	Mn(5)-O(54)	2.302(6)
Y(3)-O(24)	2.334(7)	Mn(6)-O(3)	1.882(6)
Y(3)-O(8)	2.376(7)	Mn(6)-O(24)	1.886(10)
Y(3)-O(48)	2.382(7)	Mn(6)-O(23)	1.920(9)
Y(3)-O(11)	2.434(6)	Mn(6)-N(2)	2.007(9)
Y(3)-O(7)	2.474(6)	Mn(6)-O(59)	2.221(6)
Y(3)-O(30)	2.500(7)	Mn(6)-O(56)	2.310(6)
Y(3)-O(3)	2.711(9)	Mn(7)-O(27)	1.847(7)
Y(4)-O(67)	2.266(6)	Mn(7)-O(26)	1.856(7)
Y(4)-O(55)	2.292(7)	Mn(7)-O(10)	1.907(6)
Y(4)-O(33)	2.335(8)	Mn(7)-N(3)	1.936(8)
Y(4)-O(13)	2.371(6)	Mn(7)-O(68)	2.184(8)
Y(4)-O(70)	2.400(6)	Mn(7)-O(58)	2.530(8)
Y(4)-O(16)	2.402(5)	Mn(8)-O(30)	1.882(7)
Y(4)-O(6)	2.412(6)	Mn(8)-O(29)	1.886(7)
Y(4)-O(39)	2.456(8)	Mn(8)-O(11)	1.942(7)
Y(5)-O(12)	2.239(6)	Mn(8)-N(4)	1.964(10)
Y(5)-O(14)	2.250(7)	Mn(8)-O(60)	2.188(8)
Y(5)-O(17)	2.413(6)	Mn(8)-O(62)	2.522(8)
Y(5)-O(52)	2.426(8)	Mn(9)-O(14)	1.901(7)

Y(5)-O(50)	2.441(7)	Mn(9)-O(33)	1.919(6)
Y(5)-O(16)	2.444(5)	Mn(9)-O(32)	1.927(7)
Y(5)-O(15)	2.460(6)	Mn(9)-N(5)	1.977(10)
Y(5)-O(13)	2.473(6)	Mn(9)-O(51)	2.231(6)
Y(6)-O(65)	2.298(6)	Mn(9)-O(19)	2.232(6)
Y(6)-O(57)	2.321(9)	Mn(10)-O(36)	1.897(6)
Y(6)-O(36)	2.328(9)	Mn(10)-O(12)	1.904(7)
Y(6)-O(1W)	2.413(7)	Mn(10)-O(35)	1.918(8)
Y(6)-O(15)	2.413(7)	Mn(10)-N(6)	1.956(11)
Y(6)-O(17)	2.420(6)	Mn(10)-O(18)	2.195(6)
Y(6)-O(9)	2.421(5)	Mn(10)-O(53)	2.271(6)
Y(6)-O(42)	2.456(7)	Mn(11)-O(38)	1.869(6)
Mn(1)-O(12)	1.867(6)	Mn(11)-O(39)	1.879(6)
Mn(1)-O(18)	1.936(8)	Mn(11)-O(16)	1.939(7)
Mn(1)-O(1)	1.967(7)	Mn(11)-N(7)	1.968(9)
Mn(1)-O(5)	1.974(6)	Mn(11)-O(66)	2.185(7)
Mn(1)-O(9)	2.183(6)	Mn(12)-O(42)	1.851(7)
Mn(1)-O(4)	2.244(6)	Mn(12)-O(41)	1.886(7)
Mn(2)-O(2)	1.884(5)	Mn(12)-O(17)	1.951(6)
Mn(2)-O(4)	1.908(7)	Mn(12)-N(8)	1.976(9)
Mn(2)-O(6)	1.961(7)	Mn(12)-O(64)	2.166(8)
Mn(2)-O(13)	1.970(5)	Mn(12)-O(50)	2.456(7)
O(44)-Y(1)-O(69)	85.1(3)	O(45)-Y(1)-O(5)	138.8(2)
O(44)-Y(1)-O(21)	144.8(3)	O(10)-Y(1)-O(5)	70.0(2)
O(69)-Y(1)-O(21)	75.8(2)	O(44)-Y(1)-O(27)	75.1(2)
O(44)-Y(1)-O(4)	79.0(2)	O(69)-Y(1)-O(27)	72.6(2)
O(69)-Y(1)-O(4)	146.8(3)	O(21)-Y(1)-O(27)	124.6(2)
O(21)-Y(1)-O(4)	101.4(2)	O(4)-Y(1)-O(27)	129.2(2)
O(44)-Y(1)-O(45)	72.5(3)	O(45)-Y(1)-O(27)	134.4(3)
O(69)-Y(1)-O(45)	73.5(3)	O(10)-Y(1)-O(27)	62.6(2)
O(21)-Y(1)-O(45)	73.9(2)	O(5)-Y(1)-O(27)	66.8(2)
O(4)-Y(1)-O(45)	74.0(2)	O(44)-Y(1)-O(2)	138.5(2)
O(44)-Y(1)-O(10)	136.4(2)	O(69)-Y(1)-O(2)	135.9(2)
O(69)-Y(1)-O(10)	91.5(2)	O(21)-Y(1)-O(2)	63.46(19)
O(21)-Y(1)-O(10)	74.2(2)	O(4)-Y(1)-O(2)	62.5(2)
O(4)-Y(1)-O(10)	120.0(2)	O(45)-Y(1)-O(2)	108.3(2)
O(45)-Y(1)-O(10)	147.1(2)	O(10)-Y(1)-O(2)	62.76(19)
O(44)-Y(1)-O(5)	84.9(3)	O(5)-Y(1)-O(2)	67.5(2)
O(69)-Y(1)-O(5)	139.4(2)	O(27)-Y(1)-O(2)	117.2(2)
O(21)-Y(1)-O(5)	128.4(2)	O(5)-Y(2)-O(7)	128.1(2)

O(4)-Y(1)-O(5)	68.1(2)	O(5)-Y(2)-O(2)	75.3(2)
O(11)-Y(2)-O(58)	74.4(3)	O(7)-Y(2)-O(2)	83.4(2)
O(10)-Y(2)-O(58)	66.3(2)	O(5)-Y(2)-O(3)	83.6(3)
O(5)-Y(2)-O(62)	145.4(2)	O(7)-Y(2)-O(3)	75.7(2)
O(7)-Y(2)-O(62)	74.9(2)	O(2)-Y(2)-O(3)	130.99(19)
O(2)-Y(2)-O(62)	83.7(2)	O(5)-Y(2)-O(11)	140.0(2)
O(3)-Y(2)-O(62)	130.3(3)	O(7)-Y(2)-O(11)	71.2(2)
O(11)-Y(2)-O(62)	66.4(2)	O(2)-Y(2)-O(11)	144.6(2)
O(10)-Y(2)-O(62)	75.0(2)	O(3)-Y(2)-O(11)	66.7(2)
O(58)-Y(2)-O(62)	98.4(2)	O(5)-Y(2)-O(10)	71.6(2)
O(5)-Y(2)-O(1)	63.72(19)	O(7)-Y(2)-O(10)	139.6(2)
O(7)-Y(2)-O(1)	64.3(2)	O(2)-Y(2)-O(10)	67.01(19)
O(2)-Y(2)-O(1)	65.28(17)	O(3)-Y(2)-O(10)	144.6(2)
O(3)-Y(2)-O(1)	65.71(19)	O(11)-Y(2)-O(10)	118.9(2)
O(11)-Y(2)-O(1)	120.6(2)	O(5)-Y(2)-O(58)	76.4(2)
O(10)-Y(2)-O(1)	120.6(2)	O(7)-Y(2)-O(58)	144.8(3)
O(58)-Y(2)-O(1)	131.3(2)	O(2)-Y(2)-O(58)	130.9(2)
O(62)-Y(2)-O(1)	130.34(19)	O(3)-Y(2)-O(58)	83.8(2)
O(61)-Y(3)-O(47)	84.8(3)	O(48)-Y(3)-O(7)	139.1(2)
O(61)-Y(3)-O(24)	75.5(3)	O(11)-Y(3)-O(7)	69.3(2)
O(47)-Y(3)-O(24)	143.5(3)	O(61)-Y(3)-O(30)	74.2(3)
O(61)-Y(3)-O(8)	147.5(2)	O(47)-Y(3)-O(30)	74.1(2)
O(47)-Y(3)-O(8)	80.4(3)	O(24)-Y(3)-O(30)	127.0(2)
O(24)-Y(3)-O(8)	100.2(2)	O(8)-Y(3)-O(30)	127.8(2)
O(61)-Y(3)-O(48)	75.0(3)	O(48)-Y(3)-O(30)	136.7(3)
O(47)-Y(3)-O(48)	73.4(3)	O(11)-Y(3)-O(30)	64.2(2)
O(24)-Y(3)-O(48)	72.0(3)	O(7)-Y(3)-O(30)	65.2(2)
O(8)-Y(3)-O(48)	73.0(3)	O(61)-Y(3)-O(3)	134.2(3)
O(61)-Y(3)-O(11)	91.3(3)	O(47)-Y(3)-O(3)	140.3(2)
O(47)-Y(3)-O(11)	137.5(2)	O(24)-Y(3)-O(3)	62.2(3)
O(24)-Y(3)-O(11)	74.2(2)	O(8)-Y(3)-O(3)	62.2(2)
O(8)-Y(3)-O(11)	118.9(3)	O(48)-Y(3)-O(3)	105.4(3)
O(48)-Y(3)-O(11)	145.8(3)	O(11)-Y(3)-O(3)	62.2(2)
O(61)-Y(3)-O(7)	139.4(2)	O(7)-Y(3)-O(3)	68.3(2)
O(47)-Y(3)-O(7)	86.7(3)	O(30)-Y(3)-O(3)	117.9(2)
O(24)-Y(3)-O(7)	127.9(3)	O(67)-Y(4)-O(55)	93.9(2)
O(8)-Y(3)-O(7)	68.6(2)	O(67)-Y(4)-O(33)	79.5(3)
O(70)-Y(4)-O(6)	74.5(2)	O(55)-Y(4)-O(33)	148.5(2)
O(16)-Y(4)-O(6)	118.85(18)	O(67)-Y(4)-O(13)	143.4(2)
O(67)-Y(4)-O(39)	74.0(2)	O(55)-Y(4)-O(13)	80.1(2)

O(55)-Y(4)-O(39)	71.0(2)	O(33)-Y(4)-O(13)	122.8(2)
O(33)-Y(4)-O(39)	134.2(2)	O(67)-Y(4)-O(70)	74.6(2)
O(13)-Y(4)-O(39)	69.9(2)	O(55)-Y(4)-O(70)	73.2(2)
O(70)-Y(4)-O(39)	129.8(2)	O(33)-Y(4)-O(70)	75.3(2)
O(16)-Y(4)-O(39)	64.2(2)	O(13)-Y(4)-O(70)	135.31(19)
O(6)-Y(4)-O(39)	131.7(2)	O(67)-Y(4)-O(16)	86.62(19)
O(12)-Y(5)-O(14)	117.1(2)	O(55)-Y(4)-O(16)	133.1(3)
O(12)-Y(5)-O(17)	72.5(2)	O(33)-Y(4)-O(16)	77.7(2)
O(14)-Y(5)-O(17)	142.2(2)	O(13)-Y(4)-O(16)	72.6(2)
O(12)-Y(5)-O(52)	86.1(2)	O(70)-Y(4)-O(16)	149.4(2)
O(14)-Y(5)-O(52)	137.8(2)	O(67)-Y(4)-O(6)	148.7(2)
O(17)-Y(5)-O(52)	76.2(2)	O(55)-Y(4)-O(6)	81.7(2)
O(12)-Y(5)-O(50)	136.8(2)	O(33)-Y(4)-O(6)	88.2(2)
O(14)-Y(5)-O(50)	86.8(2)	O(13)-Y(4)-O(6)	66.6(2)
O(17)-Y(5)-O(50)	67.7(2)	O(15)-Y(5)-O(13)	123.29(19)
O(52)-Y(5)-O(50)	99.8(2)	O(65)-Y(6)-O(57)	92.4(3)
O(12)-Y(5)-O(16)	142.3(2)	O(65)-Y(6)-O(36)	80.1(3)
O(14)-Y(5)-O(16)	72.3(2)	O(57)-Y(6)-O(36)	147.4(3)
O(17)-Y(5)-O(16)	124.27(18)	O(65)-Y(6)-O(1W)	73.8(2)
O(52)-Y(5)-O(16)	68.8(2)	O(57)-Y(6)-O(1W)	72.7(3)
O(50)-Y(5)-O(16)	77.1(2)	O(36)-Y(6)-O(1W)	74.8(3)
O(12)-Y(5)-O(15)	74.4(2)	O(65)-Y(6)-O(15)	143.2(3)
O(14)-Y(5)-O(15)	76.7(2)	O(57)-Y(6)-O(15)	82.3(3)
O(17)-Y(5)-O(15)	70.9(2)	O(36)-Y(6)-O(15)	121.9(2)
O(52)-Y(5)-O(15)	145.5(2)	O(1W)-Y(6)-O(15)	136.8(2)
O(50)-Y(5)-O(15)	77.4(2)	O(65)-Y(6)-O(17)	87.9(2)
O(16)-Y(5)-O(15)	140.5(3)	O(57)-Y(6)-O(17)	135.2(3)
O(12)-Y(5)-O(13)	77.6(2)	O(36)-Y(6)-O(17)	76.6(2)
O(14)-Y(5)-O(13)	73.8(2)	O(1W)-Y(6)-O(17)	148.2(3)
O(17)-Y(5)-O(13)	141.5(3)	O(15)-Y(6)-O(17)	71.6(2)
O(52)-Y(5)-O(13)	78.1(2)	O(65)-Y(6)-O(9)	149.1(2)
O(50)-Y(5)-O(13)	145.6(2)	O(57)-Y(6)-O(9)	81.6(2)
O(16)-Y(5)-O(13)	70.13(19)	O(36)-Y(6)-O(9)	88.6(2)
O(18)-Mn(1)-O(9)	91.3(3)	O(1W)-Y(6)-O(9)	75.5(2)
O(1)-Mn(1)-O(9)	90.3(3)	O(15)-Y(6)-O(9)	66.3(2)
O(5)-Mn(1)-O(9)	98.6(2)	O(17)-Y(6)-O(9)	117.53(18)
O(12)-Mn(1)-O(4)	96.6(2)	O(65)-Y(6)-O(42)	74.0(3)
O(18)-Mn(1)-O(4)	90.4(3)	O(57)-Y(6)-O(42)	73.1(2)
O(1)-Mn(1)-O(4)	87.9(3)	O(36)-Y(6)-O(42)	132.9(2)
O(5)-Mn(1)-O(4)	79.7(2)	O(1W)-Y(6)-O(42)	131.2(2)

O(9)-Mn(1)-O(4)	177.6(3)	O(15)-Y(6)-O(42)	69.7(2)
O(3)-Mn(3)-O(8)	88.6(3)	O(17)-Y(6)-O(42)	64.0(2)
O(3)-Mn(3)-O(15)	173.6(3)	O(9)-Y(6)-O(42)	131.4(2)
O(8)-Mn(3)-O(15)	90.3(3)	O(12)-Mn(1)-O(18)	86.9(3)
O(3)-Mn(3)-O(9)	95.6(3)	O(12)-Mn(1)-O(1)	94.6(3)
O(8)-Mn(3)-O(9)	173.9(3)	O(18)-Mn(1)-O(1)	177.8(2)
O(15)-Mn(3)-O(9)	85.1(3)	O(12)-Mn(1)-O(5)	175.8(3)
O(3)-Mn(3)-O(56)	82.7(2)	O(18)-Mn(1)-O(5)	91.4(3)
O(8)-Mn(3)-O(56)	97.0(3)	O(1)-Mn(1)-O(5)	87.0(3)
O(15)-Mn(3)-O(56)	103.7(2)	O(12)-Mn(1)-O(9)	85.2(2)
O(9)-Mn(3)-O(56)	88.0(3)	O(1)-Mn(4)-O(8)	87.2(3)
O(3)-Mn(3)-O(1)	84.5(2)	O(6)-Mn(4)-O(8)	177.1(3)
O(8)-Mn(3)-O(1)	88.5(3)	O(21)-Mn(5)-O(2)	89.3(3)
O(15)-Mn(3)-O(1)	89.2(2)	O(21)-Mn(5)-O(20)	173.6(3)
O(9)-Mn(3)-O(1)	87.5(3)	O(2)-Mn(5)-O(20)	97.0(3)
O(56)-Mn(3)-O(1)	165.9(2)	O(21)-Mn(5)-N(1)	84.5(3)
O(14)-Mn(4)-O(19)	88.2(3)	O(2)-Mn(5)-N(1)	170.8(3)
O(14)-Mn(4)-O(7)	175.2(3)	O(20)-Mn(5)-N(1)	89.1(3)
O(19)-Mn(4)-O(7)	89.4(3)	O(21)-Mn(5)-O(63)	89.5(3)
O(14)-Mn(4)-O(1)	94.5(3)	O(2)-Mn(5)-O(63)	95.9(2)
O(19)-Mn(4)-O(1)	177.1(3)	O(20)-Mn(5)-O(63)	91.0(3)
O(7)-Mn(4)-O(1)	87.8(3)	N(1)-Mn(5)-O(63)	90.8(3)
O(14)-Mn(4)-O(6)	85.4(2)	O(21)-Mn(5)-O(54)	90.0(3)
O(19)-Mn(4)-O(6)	91.2(3)	O(2)-Mn(5)-O(54)	80.3(2)
O(7)-Mn(4)-O(6)	98.8(2)	O(20)-Mn(5)-O(54)	89.9(3)
O(1)-Mn(4)-O(6)	90.0(3)	N(1)-Mn(5)-O(54)	92.9(3)
O(14)-Mn(4)-O(8)	95.7(2)	O(63)-Mn(5)-O(54)	176.2(2)
O(19)-Mn(4)-O(8)	91.5(3)	O(3)-Mn(6)-O(24)	88.3(3)
O(7)-Mn(4)-O(8)	80.2(2)	O(3)-Mn(6)-O(23)	96.9(3)
O(26)-Mn(7)-N(3)	92.2(3)	O(24)-Mn(6)-O(23)	174.6(3)
O(10)-Mn(7)-N(3)	169.4(3)	O(3)-Mn(6)-N(2)	170.5(5)
O(27)-Mn(7)-O(68)	92.5(3)	O(24)-Mn(6)-N(2)	84.2(5)
O(26)-Mn(7)-O(68)	91.6(3)	O(23)-Mn(6)-N(2)	90.4(5)
O(10)-Mn(7)-O(68)	95.3(3)	O(3)-Mn(6)-O(59)	96.4(2)
N(3)-Mn(7)-O(68)	87.1(3)	O(24)-Mn(6)-O(59)	88.9(3)
O(27)-Mn(7)-O(58)	87.2(3)	O(23)-Mn(6)-O(59)	92.0(3)
O(26)-Mn(7)-O(58)	89.6(3)	N(2)-Mn(6)-O(59)	89.3(3)
O(10)-Mn(7)-O(58)	73.4(2)	O(3)-Mn(6)-O(56)	79.9(2)
N(3)-Mn(7)-O(58)	104.1(3)	O(24)-Mn(6)-O(56)	88.6(3)
O(68)-Mn(7)-O(58)	168.7(2)	O(23)-Mn(6)-O(56)	90.9(3)

O(30)-Mn(8)-O(29)	173.4(3)	N(2)-Mn(6)-O(56)	94.0(3)
O(30)-Mn(8)-O(11)	86.6(3)	O(59)-Mn(6)-O(56)	175.6(3)
O(29)-Mn(8)-O(11)	97.4(3)	O(27)-Mn(7)-O(26)	174.2(3)
O(30)-Mn(8)-N(4)	84.1(4)	O(27)-Mn(7)-O(10)	85.6(3)
O(29)-Mn(8)-N(4)	91.6(4)	O(26)-Mn(7)-O(10)	98.0(3)
O(11)-Mn(8)-N(4)	170.4(4)	O(27)-Mn(7)-N(3)	84.0(3)
O(30)-Mn(8)-O(60)	94.3(3)	O(14)-Mn(9)-O(19)	78.4(3)
O(29)-Mn(8)-O(60)	90.6(3)	O(33)-Mn(9)-O(19)	90.8(2)
O(11)-Mn(8)-O(60)	95.3(3)	O(32)-Mn(9)-O(19)	91.7(3)
N(4)-Mn(8)-O(60)	87.9(4)	N(5)-Mn(9)-O(19)	97.2(3)
O(30)-Mn(8)-O(62)	87.0(3)	O(51)-Mn(9)-O(19)	171.6(3)
O(29)-Mn(8)-O(62)	89.1(3)	O(36)-Mn(10)-O(12)	90.4(3)
O(11)-Mn(8)-O(62)	73.1(3)	O(36)-Mn(10)-O(35)	171.2(4)
N(4)-Mn(8)-O(62)	103.8(4)	O(12)-Mn(10)-O(35)	98.1(3)
O(60)-Mn(8)-O(62)	168.3(3)	O(36)-Mn(10)-N(6)	83.0(4)
O(14)-Mn(9)-O(33)	90.7(3)	O(12)-Mn(10)-N(6)	172.6(4)
O(14)-Mn(9)-O(32)	96.5(3)	O(35)-Mn(10)-N(6)	88.6(4)
O(33)-Mn(9)-O(32)	172.8(4)	O(36)-Mn(10)-O(18)	92.9(2)
O(14)-Mn(9)-N(5)	172.4(3)	O(12)-Mn(10)-O(18)	78.9(3)
O(33)-Mn(9)-N(5)	83.1(4)	O(35)-Mn(10)-O(18)	90.9(3)
O(32)-Mn(9)-N(5)	89.9(4)	N(6)-Mn(10)-O(18)	97.9(3)
O(14)-Mn(9)-O(51)	93.5(3)	O(36)-Mn(10)-O(53)	88.6(2)
O(33)-Mn(9)-O(51)	91.6(3)	O(12)-Mn(10)-O(53)	92.5(3)
O(32)-Mn(9)-O(51)	87.0(3)	O(35)-Mn(10)-O(53)	88.9(3)
N(5)-Mn(9)-O(51)	91.1(3)	N(6)-Mn(10)-O(53)	90.8(3)
O(42)-Mn(12)-O(64)	90.7(3)	O(18)-Mn(10)-O(53)	171.3(3)
O(41)-Mn(12)-O(64)	90.6(3)	O(38)-Mn(11)-O(39)	174.1(4)
O(17)-Mn(12)-O(64)	96.3(3)	O(38)-Mn(11)-O(16)	98.6(3)
N(8)-Mn(12)-O(64)	86.4(4)	O(39)-Mn(11)-O(16)	85.1(3)
O(42)-Mn(12)-O(50)	90.0(3)	O(38)-Mn(11)-N(7)	91.7(3)
O(41)-Mn(12)-O(50)	89.4(2)	O(39)-Mn(11)-N(7)	84.2(3)
O(17)-Mn(12)-O(50)	74.7(3)	O(16)-Mn(11)-N(7)	168.3(3)
N(8)-Mn(12)-O(50)	102.7(4)	O(38)-Mn(11)-O(66)	91.1(3)
O(64)-Mn(12)-O(50)	170.9(3)	O(39)-Mn(11)-O(66)	93.0(3)
Mn(1)-O(1)-Mn(4)	167.6(3)	O(16)-Mn(11)-O(66)	96.3(3)
Mn(1)-O(1)-Mn(2)	90.1(3)	N(7)-Mn(11)-O(66)	88.8(3)
Mn(4)-O(1)-Mn(2)	89.3(2)	O(42)-Mn(12)-O(41)	175.7(4)
Mn(1)-O(1)-Mn(3)	89.3(2)	O(42)-Mn(12)-O(17)	85.6(3)
Mn(4)-O(1)-Mn(3)	90.1(3)	O(41)-Mn(12)-O(17)	98.4(3)
Mn(2)-O(1)-Mn(3)	174.4(3)	O(42)-Mn(12)-N(8)	84.7(4)

Mn(1)-O(1)-Y(2)	96.5(2)	O(41)-Mn(12)-N(8)	91.2(3)
Mn(4)-O(1)-Y(2)	95.8(2)	O(17)-Mn(12)-N(8)	170.0(4)
Mn(2)-O(1)-Y(2)	92.89(18)	Y(2)-O(5)-Y(1)	101.4(2)
Mn(3)-O(1)-Y(2)	92.7(2)	Mn(2)-O(6)-Mn(4)	91.9(2)
Mn(2)-O(2)-Mn(5)	108.0(3)	Mn(2)-O(6)-Y(4)	100.3(3)
Mn(2)-O(2)-Y(2)	118.0(2)	Mn(4)-O(6)-Y(4)	111.4(2)
Mn(5)-O(2)-Y(2)	130.9(3)	Mn(4)-O(7)-Y(2)	111.3(3)
Mn(2)-O(2)-Y(1)	97.9(3)	Mn(4)-O(7)-Y(3)	106.8(2)
Mn(5)-O(2)-Y(1)	96.8(2)	Y(2)-O(7)-Y(3)	101.3(2)
Y(2)-O(2)-Y(1)	93.30(18)	Mn(3)-O(8)-Mn(4)	93.4(3)
Mn(6)-O(3)-Mn(3)	109.2(3)	Mn(3)-O(8)-Y(3)	109.7(3)
Mn(6)-O(3)-Y(2)	130.2(3)	Mn(4)-O(8)-Y(3)	101.0(2)
Mn(3)-O(3)-Y(2)	117.1(3)	Mn(3)-O(9)-Mn(1)	92.8(2)
Mn(6)-O(3)-Y(3)	97.7(3)	Mn(3)-O(9)-Y(6)	99.7(3)
Mn(3)-O(3)-Y(3)	97.8(3)	Mn(1)-O(9)-Y(6)	112.4(3)
Y(2)-O(3)-Y(3)	93.3(2)	Mn(7)-O(10)-Y(1)	101.9(3)
Mn(2)-O(4)-Mn(1)	92.7(3)	Mn(7)-O(10)-Y(2)	120.9(3)
Mn(2)-O(4)-Y(1)	109.1(3)	Y(1)-O(10)-Y(2)	99.03(19)
Mn(1)-O(4)-Y(1)	101.8(2)	Mn(8)-O(11)-Y(3)	100.2(3)
Mn(1)-O(5)-Y(2)	112.0(3)	Mn(8)-O(11)-Y(2)	120.7(3)
Mn(1)-O(5)-Y(1)	107.2(3)	Y(3)-O(11)-Y(2)	99.6(2)
Y(5)-O(17)-Y(6)	102.4(2)	Mn(1)-O(12)-Mn(10)	102.4(3)
Mn(1)-O(18)-Mn(10)	90.5(3)	Mn(1)-O(12)-Y(5)	122.8(3)
Mn(4)-O(19)-Mn(9)	89.3(3)	Mn(10)-O(12)-Y(5)	132.7(3)
Mn(5)-O(21)-Y(1)	110.4(3)	Mn(2)-O(13)-Y(4)	101.5(3)
Mn(6)-O(24)-Y(3)	111.7(3)	Mn(2)-O(13)-Y(5)	121.0(3)
Mn(7)-O(27)-Y(1)	101.1(3)	Y(4)-O(13)-Y(5)	101.9(2)
Mn(8)-O(30)-Y(3)	99.7(3)	Mn(4)-O(14)-Mn(9)	102.6(4)
Mn(9)-O(33)-Y(4)	116.2(3)	Mn(4)-O(14)-Y(5)	123.2(3)
Mn(10)-O(36)-Y(6)	117.3(3)	Mn(9)-O(14)-Y(5)	132.0(3)
Mn(11)-O(39)-Y(4)	101.7(3)	Mn(3)-O(15)-Y(6)	100.0(3)
Mn(12)-O(42)-Y(6)	102.7(4)	Mn(3)-O(15)-Y(5)	122.3(3)
Y(5)-O(50)-Mn(12)	99.8(3)	Y(6)-O(15)-Y(5)	101.2(3)
Mn(2)-O(54)-Mn(5)	85.8(2)	Mn(11)-O(16)-Y(4)	101.8(2)
Mn(3)-O(56)-Mn(6)	85.8(2)	Mn(11)-O(16)-Y(5)	118.2(3)
Y(2)-O(58)-Mn(7)	99.1(2)	Y(4)-O(16)-Y(5)	101.83(19)
Y(2)-O(62)-Mn(8)	99.4(2)	Mn(12)-O(17)-Y(5)	117.8(3)
Mn(12)-O(17)-Y(6)	101.0(3)		

Ab Initio calculations of the local magnetic properties on Dy sites in 1-Dy and 2-Dy.

Computational details
All ab initio calculations were done with MOLCAS 7.4. program package. All basis sets were taken from the ANO-RCC basis set library available in MOLCAS. The following contractions were used for all calculations:

Dy – 8s7p5d4f2g1h
La – La.ECP.deGraaf.0s.0s.0e-La(LaMnO3).
Zn – Zn.ECP.Lopez-Moraza.0s.0s.0e-AIMP-KZnF3.
N, O – 4s3p2d. (only for the first coordinated atoms, which make a bond with Dy)
C – 4s3p2d. (only for the atoms which are directly bonded to the first coordination sphere of O and N)
N,O, C – 3s2p. (for distant atoms)
H – 2s. (for distant atoms)

Active space of the CASSCF method included 9 electrons in 7 orbitals.
The **spin orbit interaction** was computed by mixing of 21 sextets, 128 quartets and 32 doublet spin free states.

The structure of the calculated Dy^{3+} fragments is listed below.
Centers coming from the same triade are marked with the same colour (green or yellow).
In all model fragments, neighboring metal ions were modeled by diamagnetic ab initio model potentials available in MOLCAS. Dy ions were modeled by La-AIMP, while the neighboring Mn- by Zn- AIMP.

Complex 1-Dy

Structure of the calculated Dy fragments

a) b)

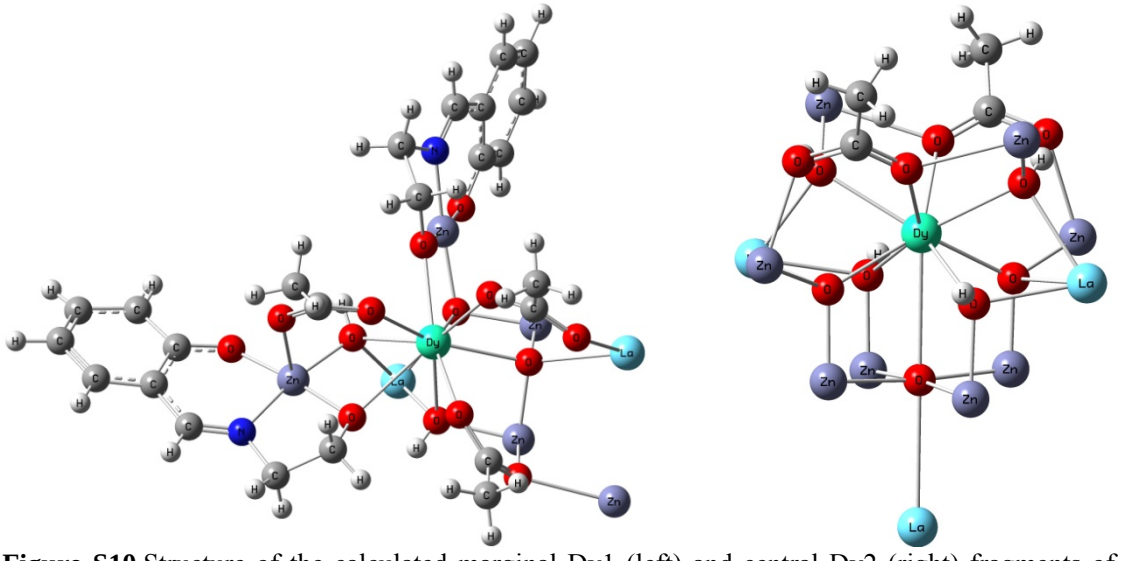

Figure S10. Structure of the calculated marginal Dy1 (left) and central Dy2 (right) fragments of the first triade (Dy1, Dy2 and Dy6). The structure of the marginal Dy6 fragment is similar to the Dy1. The fragments of the second triade (marginal Dy3 and Dy5 and central Dy4) have similar structures. Even if these Dy fragments have structural similarities, every Dy center was calculated ab initio.

Table S2. Energies of the lowest spin free states of the Dy^{3+} sites.(cm^{-1})

Spin Multiplicity	Dy1	Dy2	Dy3	Dy4	Dy5	Dy6

6	0.000	0.000	0.000	0.000	0.000	0.000
	35.884	5.930	35.885	5.918	35.746	53.032
	224.614	43.412	224.678	43.507	224.183	211.272
	318.924	59.694	318.982	59.771	318.375	306.008
	326.144	165.800	326.224	165.803	325.350	338.769
	357.923	235.792	357.930	235.812	357.612	391.629
	403.692	291.579	403.758	291.591	402.926	400.835
	482.170	300.813	482.166	300.803	482.049	469.249
	501.782	351.924	501.762	351.906	501.857	486.087
	771.998	536.037	771.951	536.231	772.343	713.680
	792.701	538.440	792.656	538.628	793.019	739.710
	7691.438	7531.119	7691.495	7531.165	7690.928	7692.176
	7727.893	7617.303	7727.887	7617.342	7727.826	7719.464
	7800.580	7663.306	7800.578	7663.327	7800.464	7781.558
	7830.712	7669.071	7830.745	7669.089	7830.384	7846.853
	7922.586	7711.322	7922.582	7711.389	7922.351	7894.279
	7935.911	7741.500	7935.919	7741.606	7935.622	7915.602
	7984.267	7798.512	7984.271	7798.586	7984.195	7969.238
	34842.346	34659.701	34842.325	34659.671	34842.182	34876.046
	35084.822	35008.734	35084.966	35008.698	35083.513	35092.985
	35432.631	35149.820	35432.553	35150.051	35433.159	35365.376
4	24948.724	24858.868	24948.747	24858.897	24948.860	24949.146
	24955.632	24860.705	24955.653	24860.734	24955.755	24955.948
	25003.055	24879.491	25003.105	24879.521	25003.004	24991.772
	25006.665	24892.730	25006.739	24892.777	25006.511	25010.998
	25008.771	24910.195	25008.812	24910.250	25008.659	25021.674
	25025.330	24924.283	25025.351	24924.317	25025.505	25031.126
	25047.037	24937.235	25047.060	24937.286	25047.342	25053.349
	25083.465	24945.471	25083.490	24945.505	25083.707	25085.409
	25100.462	24975.585	25100.468	24975.631	25101.028	25100.600
	25146.022	24999.566	25146.051	24999.593	25146.180	25125.647
	25158.855	25000.778	25158.868	25000.854	25159.198	25139.857
	25189.799	25023.208	25189.819	25023.298	25190.061	25167.706
	25234.659	25024.521	25234.687	25024.600	25234.649	25212.067
	25250.554	25156.877	25250.583	25156.925	25250.707	25260.251
	25299.778	25180.766	25299.818	25180.813	25299.901	25301.764
	25341.898	25191.458	25341.920	25191.514	25342.008	25335.465
	25364.286	25224.361	25364.309	25224.434	25364.504	25354.816
	25374.207	25238.717	25374.209	25238.759	25374.823	25366.566
	25397.832	25249.570	25397.849	25249.609	25397.860	25392.442
	25404.271	25257.912	25404.274	25257.974	25404.691	25400.047
	25415.029	25263.512	25415.060	25263.573	25415.273	25419.112
	25444.545	25290.376	25444.582	25290.426	25444.671	25448.368
	25462.528	25294.153	25462.554	25294.196	25462.790	25459.018
	25480.589	25331.725	25480.607	25331.796	25480.461	25472.551
	25500.631	25359.714	25500.658	25359.748	25500.513	25489.044
	25510.134	25366.818	25510.148	25366.847	25510.155	25505.888
	25543.665	25376.266	25543.674	25376.307	25543.573	25527.432
	25566.904	25377.774	25566.917	25377.814	25566.879	25550.275
	25604.367	25410.882	25604.399	25410.929	25604.467	25585.528
	...	...	...	...	...	...
2	37380.803	37267.403	37380.837	37267.448	37380.178	37370.888
	37386.249	37271.163	37386.288	37271.210	37385.681	37377.969
	37407.892	37292.239	37407.926	37292.279	37407.334	37402.345
	37410.176	37293.894	37410.218	37293.937	37409.679	37406.780
	37436.459	37307.695	37436.465	37307.737	37435.912	37429.875
	37473.990	37317.251	37473.999	37317.294	37473.427	37463.967
	37545.730	37348.308	37545.746	37348.342	37545.097	37552.384
	37560.951	37375.163	37560.969	37375.207	37560.301	37558.150
	37586.157	37410.779	37586.165	37410.833	37585.798	37581.053
	37602.890	37446.163	37602.907	37446.240	37602.449	37594.842
	37616.381	37462.265	37616.404	37462.332	37615.633	37601.647

	37623.350	37477.723	37623.364	37477.778	37622.853	37609.632
	37699.879	37487.864	37699.893	37487.904	37699.319	37691.276
	37736.780	37515.689	37736.794	37515.729	37736.221	37730.567
	37741.146	37531.464	37741.167	37531.509	37740.520	37733.139
	37761.633	37536.315	37761.652	37536.363	37760.953	37755.295
	37764.001	37539.693	37764.022	37539.732	37763.305	37758.843
	39084.153	38967.708	39084.177	38967.748	39083.683	39069.772
	39099.665	38973.468	39099.691	38973.506	39099.081	39084.001
	39119.091	38977.758	39119.147	38977.800	39118.575	39123.809
	39136.311	38983.609	39136.335	38983.639	39135.869	39126.941
	39154.116	39033.776	39154.132	39033.822	39153.560	39152.154
	39174.756	39036.269	39174.762	39036.316	39174.253	39166.765
	39235.700	39037.871	39235.713	39037.894	39235.363	39244.836
	39240.228	39064.607	39240.247	39064.646	39239.766	39250.809
	39285.806	39099.930	39285.817	39099.960	39285.354	39282.249
	39329.913	39128.696	39329.920	39128.789	39329.525	39316.142
	39339.708	39130.147	39339.719	39130.241	39339.150	39324.542
	39348.641	39138.881	39348.659	39138.932	39347.948	39330.193
	39364.258	39140.461	39364.278	39140.514	39363.615	39348.306
	39385.149	39157.292	39385.167	39157.328	39384.437	39376.023
	39392.031	39163.045	39392.051	39163.080	39391.288	39380.299
	...	...	...	...	...	...

Table S3. Energies of the lowest spin-orbit Kramers doublets states of the Dy^{3+} sites.(cm^{-1})

	Dy1	Dy2	Dy3	Dy4	Dy5	Dy6
	0.000	0.000	0.000	0.000	0.000	0.000
	135.009	90.303	135.042	90.347	134.755	121.455
	195.996	115.056	196.075	115.117	195.501	184.144
	252.697	158.733	252.762	158.791	252.293	245.622
	292.383	197.267	292.425	197.328	292.203	284.242
	344.744	266.794	344.780	266.837	344.631	319.869
	392.816	296.076	392.780	296.096	393.242	356.414
	647.649	482.617	647.614	482.823	647.971	570.612
	3644.461	3574.865	3644.470	3574.885	3644.278	3623.059
	3675.042	3604.027	3675.057	3604.056	3674.934	3691.064
	3739.035	3681.053	3739.119	3681.084	3738.474	3739.394
	3780.821	3733.487	3780.872	3733.544	3780.557	3771.966
	3853.469	3789.629	3853.496	3789.649	3853.364	3824.203
	3939.237	3816.364	3939.252	3816.460	3939.278	3896.581
	4030.611	3877.368	4030.572	3877.549	4030.994	3962.911
	6175.674	6101.547	6175.687	6101.571	6175.607	6172.618
	6207.793	6142.782	6207.829	6142.813	6207.503	6207.609
	6276.568	6223.975	6276.638	6224.021	6276.037	6265.842
	6337.018	6284.889	6337.040	6284.912	6336.953	6315.078
	6448.131	6339.602	6448.172	6339.748	6447.978	6396.207
	6489.726	6339.982	6489.682	6340.082	6490.180	6448.477
	8136.913	8062.283	8136.938	8062.315	8136.798	8130.770
	8171.178	8104.189	8171.210	8104.231	8170.936	8162.202
	8233.869	8208.198	8233.921	8208.229	8233.567	8220.966
	8386.743	8275.642	8386.782	8275.776	8386.556	8336.372
	8416.177	8282.823	8416.145	8282.895	8416.568	8387.097
	9639.100	9570.835	9639.130	9570.874	9638.962	9627.544
	9728.022	9684.141	9728.060	9684.168	9727.757	9724.683
	9836.173	9782.291	9836.218	9782.348	9835.969	9814.562
	9946.454	9809.282	9946.434	9809.415	9946.774	9896.224
	10098.143	10015.817	10098.188	10015.861	10097.880	10072.670
	10106.608	10019.823	10106.618	10019.879	10106.541	10099.858
	10142.631	10065.327	10142.669	10065.397	10142.393	10125.533
	10193.294	10067.377	10193.311	10067.412	10193.122	10165.001
	10238.833	10102.952	10238.839	10103.035	10238.848	10210.022
	10275.431	10168.101	10275.441	10168.195	10275.362	10242.849

	10819.000	10747.418	10819.021	10747.441	10818.879	10815.170
	10925.511	10876.680	10925.578	10876.711	10925.164	10918.122
	11148.346	11025.296	11148.323	11025.449	11148.686	11091.438
	11533.783	11439.736	11533.813	11439.777	11533.612	11517.631
	11591.558	11475.231	11591.580	11475.308	11591.456	11566.563
	11610.221	11491.721	11610.230	11491.791	11610.212	11581.475
	11618.699	11523.487	11618.714	11523.553	11618.725	11594.454
	11641.066	11535.169	11641.089	11535.241	11640.982	11615.364
	13469.107	13381.352	13469.132	13381.414	13469.040	13446.279
	13517.106	13412.907	13517.128	13412.967	13516.980	13494.492
	13546.427	13448.947	13546.444	13449.017	13546.343	13522.052
	13572.739	13464.177	13572.760	13464.250	13572.694	13549.307
	14937.601	14852.996	14937.625	14853.058	14937.509	14913.119
	14982.379	14866.672	14982.399	14866.741	14982.280	14960.486
	14996.233	14901.716	14996.251	14901.785	14996.167	14972.899
	15826.843	15733.880	15826.869	15733.944	15826.719	15806.509
	15846.647	15740.557	15846.663	15740.629	15846.603	15820.572
	16369.335	16268.637	16369.354	16268.707	16369.273	16344.354
	24583.267	24508.212	24583.301	24508.270	24583.421	24565.820
	24621.363	24603.819	24621.390	24603.877	24621.497	24600.164
	24724.008	24630.967	24724.046	24631.021	24724.059	24706.252
	24771.094	24657.009	24771.127	24657.062	24771.175	24748.102
	24883.296	24778.611	24883.318	24778.686	24883.450	24861.806
	25188.338	25126.357	25188.363	25126.407	25188.131	25145.665
	25226.675	25134.046	25226.757	25134.092	25226.341	25233.160
	25245.032	25197.559	25245.061	25197.603	25244.933	25246.874
	25274.309	25221.160	25274.325	25221.193	25274.430	25286.150
	25355.608	25245.909	25355.622	25245.977	25355.794	25336.502
	25436.194	25314.561	25436.232	25314.690	25436.051	25409.049
	25470.697	25327.452	25470.727	25327.499	25470.673	25426.120
	25516.943	25354.348	25516.927	25354.440	25517.254	25471.521
	27281.193	27208.729	27281.218	27208.755	27281.322	27283.019
	27346.481	27277.221	27346.527	27277.275	27346.523	27335.638
	27377.729	27304.595	27377.777	27304.660	27377.788	27361.578
	27410.859	27337.381	27410.895	27337.448	27411.001	27388.492
	27453.030	27356.223	27453.063	27356.289	27453.196	27424.300
	27523.243	27396.306	27523.241	27396.434	27523.749	27480.987
	27550.381	27515.802	27550.371	27515.850	27550.936	27518.085
	27580.880	27517.959	27580.935	27518.015	27581.090	27588.314
	...	...	...	...	...	...

Table S4. Main values of the *g* tensor of the lowest Kramers doublet on Dy^{3+} sites in complex 1-Dy.

	Dy1	Dy2	Dy3	Dy4	Dy5	Dy6
gx	0.1388	0.0717	0.1387	0.0716	0.1388	0.1295
gy	0.2174	0.0861	0.2197	0.0849	0.2184	0.2264
gz	18.8602	19.8561	18.8950	19.4853	18.7957	19.1599

Table S5. Relative angles between main anisotropy axes on Dy sites in complex 1-Dy.

	Dy1	Dy2	Dy3	Dy4	Dy5	Dy6
Dy1	0.00	11.35	71.23	80.00	70.16	12.08
Dy2	11.35	0.00	79.47	89.13	80.00	20.58
Dy3	71.23	79.47	0.00	11.55	13.06	59.44
Dy4	80.00	89.13	11.55	0.00	11.43	68.68
Dy5	70.16	80.00	13.06	11.43	0.00	59.41
Dy6	12.08	20.58	59.44	68.68	59.41	0.00

Complex 2-Dy

Structure of the calculated Dy fragments

a) b)

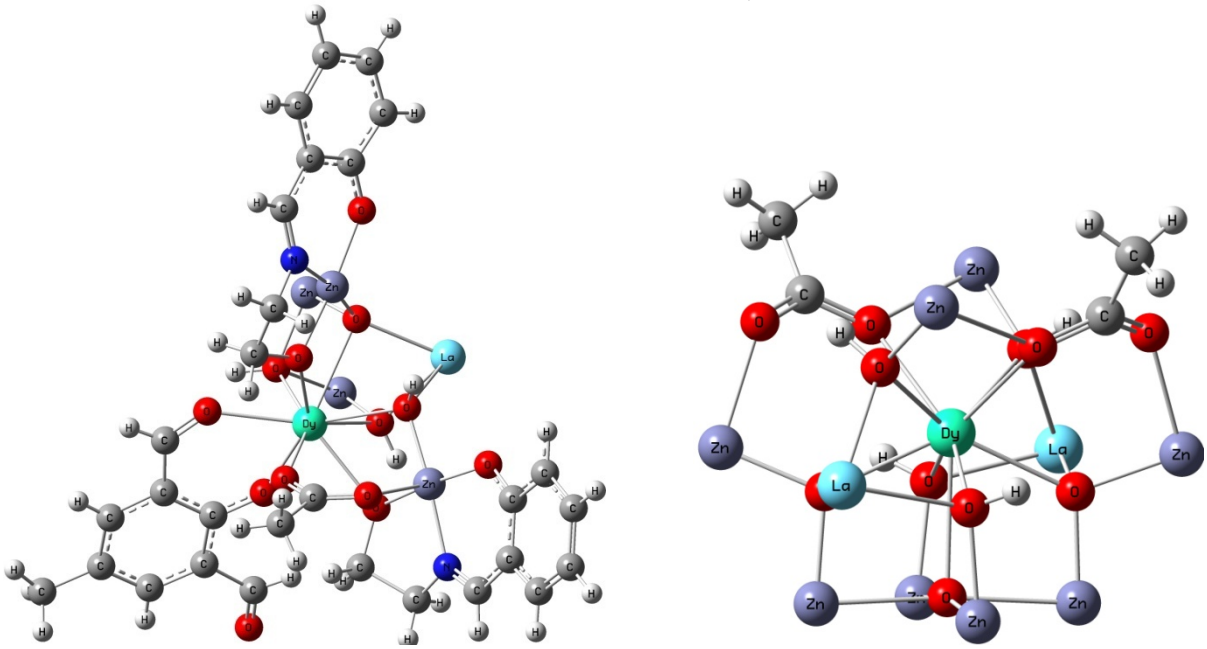

Figure S11. Structure of the calculated marginal Dy1 (left) and central Dy2 (right) fragments of the first triade (Dy1, Dy2 and Dy3). The structure of the marginal Dy3 fragment is similar to the Dy1. The fragments of the second triade (marginal Dy4 and Dy5 and central Dy6) have similar structures. Even if these Dy fragments have structural similarities, every Dy center was calculated ab initio.

Table S6. Energies of the lowest spin free states of the Dy^{3+} sites.(cm^{-1})

Spin Multiplicity	Dy1	Dy2	Dy3	Dy4	Dy5	Dy6
6	0.000	0.000	0.000	0.000	0.000	0.000
	21.408	40.874	22.633	40.078	6.875	35.982
	276.686	75.608	221.556	192.234	58.026	193.927
	317.180	103.226	262.915	307.254	121.861	295.076
	466.380	121.138	374.776	356.132	158.232	354.888
	578.062	244.044	479.844	384.700	276.979	397.698
	600.229	259.854	511.292	458.088	382.205	482.244
	811.115	325.476	644.289	529.342	463.084	520.246
	819.267	364.265	653.876	544.981	514.573	545.984
	877.518	656.025	776.011	847.963	696.714	844.705
	880.098	657.297	778.248	859.129	705.593	856.314
	7803.720	7567.903	7741.497	7707.201	7594.331	7709.564
	7834.863	7663.500	7762.858	7740.824	7673.236	7741.197
	7943.929	7667.444	7837.737	7813.012	7732.219	7814.339
	7998.238	7681.219	7910.094	7882.715	7744.946	7878.462
	8036.920	7770.268	7942.801	7958.166	7771.791	7964.028
	8083.822	7792.070	7984.751	7979.560	7894.960	7977.366
	8123.199	7850.615	8030.494	8018.049	7921.703	8022.604
	34728.033	34702.261	34765.222	34785.322	34590.009	34766.067
	35238.218	34969.635	35125.180	35122.564	35229.878	35157.919
	35781.114	35324.517	35605.364	35545.645	35289.175	35541.900
4	24986.733	24899.622	24951.001	24948.512	24897.085	24945.750
	24987.750	24902.196	24953.121	24953.318	24904.125	24950.861
	25122.278	24921.616	25050.708	25023.982	24908.884	25028.281
	25135.896	24930.129	25070.397	25036.556	24923.080	25037.678
	25182.830	24950.134	25099.259	25074.680	24977.620	25078.939
	25228.089	24960.831	25152.090	25091.108	24990.069	25105.185
	25251.480	24982.019	25169.044	25095.499	25020.495	25105.769

	25270.794	24992.529	25194.642	25139.255	25023.816	25139.997
	25273.464	25002.813	25200.269	25151.840	25091.566	25148.912
	25324.103	25019.512	25231.066	25178.592	25097.005	25190.343
	25335.390	25028.710	25236.568	25189.900	25130.898	25196.179
	25354.512	25095.785	25253.435	25222.197	25164.548	25233.062
	25355.024	25104.863	25260.319	25240.439	25184.396	25253.013
	25406.567	25217.080	25322.918	25296.343	25258.392	25299.874
	25430.237	25246.542	25354.664	25349.118	25271.469	25353.373
	25456.284	25255.980	25375.301	25364.311	25304.962	25362.389
	25477.189	25267.974	25394.675	25380.149	25316.646	25383.006
	25482.209	25296.253	25405.412	25396.144	25321.662	25400.129
	25506.031	25298.788	25429.790	25407.441	25328.429	25406.226
	25531.065	25313.466	25473.804	25435.565	25341.698	25438.789
	25539.965	25318.132	25476.004	25462.341	25355.999	25465.015
	25559.316	25324.075	25486.455	25483.504	25359.433	25482.717
	25588.651	25338.380	25510.274	25488.558	25367.996	25490.000
	25591.407	25368.453	25515.732	25519.795	25416.131	25517.034
	25632.866	25374.459	25559.458	25534.826	25418.312	25528.746
	25638.011	25399.934	25569.569	25546.935	25431.225	25545.424
	25670.413	25419.687	25600.316	25569.235	25437.934	25559.753
	25675.811	25421.508	25604.944	25580.066	25443.522	25579.086
	25705.964	25428.167	25630.391	25594.885	25482.268	25596.152
	...	...	...	...	...	...
2	37527.625	37311.859	37453.125	37411.457	37354.698	37416.840
	37542.228	37316.894	37472.657	37425.537	37357.282	37427.270
	37566.041	37328.162	37484.959	37430.808	37361.057	37446.478
	37593.621	37334.111	37501.729	37442.925	37361.669	37457.481
	37602.971	37371.297	37506.192	37477.071	37416.872	37487.634
	37626.063	37383.407	37542.765	37518.386	37430.250	37527.116
	37650.874	37422.640	37568.837	37568.630	37436.239	37574.023
	37692.677	37427.460	37617.119	37586.293	37445.951	37582.666
	37704.306	37480.460	37627.389	37600.974	37506.481	37599.963
	37731.643	37496.139	37651.858	37619.115	37559.248	37626.834
	37750.897	37531.621	37667.507	37673.174	37584.298	37683.334
	37765.514	37533.362	37685.898	37677.049	37591.748	37686.710
	37774.902	37541.763	37697.622	37721.898	37600.143	37721.848
	37829.974	37578.380	37751.221	37760.764	37604.023	37757.401
	37840.296	37599.830	37760.544	37765.407	37605.996	37762.314
	37867.014	37602.333	37787.960	37781.406	37611.745	37784.368
	37872.054	37603.668	37792.375	37792.891	37629.066	37794.223
	39176.519	39019.278	39115.527	39093.697	39026.087	39096.503
	39185.726	39023.285	39128.479	39104.554	39034.015	39106.247
	39259.508	39025.319	39179.433	39159.361	39038.735	39173.383
	39300.604	39033.910	39219.895	39164.199	39047.391	39175.704
	39310.061	39090.147	39227.865	39200.875	39110.868	39206.834
	39346.049	39092.426	39244.652	39227.176	39117.040	39231.432
	39351.793	39098.831	39254.945	39259.418	39137.313	39257.158
	39383.552	39110.128	39303.228	39271.547	39158.139	39276.902
	39386.532	39158.847	39306.630	39308.869	39206.723	39305.627
	39437.165	39190.450	39358.628	39348.342	39213.660	39348.068
	39442.178	39195.294	39363.499	39365.454	39216.990	39365.032
	39476.719	39211.640	39393.058	39395.734	39254.727	39400.505
	39478.281	39215.804	39394.166	39398.473	39264.961	39403.416
	39495.877	39234.073	39413.670	39405.998	39292.339	39411.565
	39496.841	39235.149	39414.138	39411.561	39293.351	39416.251
	...	...	...	...	...	...

Table S7. Energies of the lowest spin-orbit Kramers doublets states of the Dy^{3+} sites.(cm^{-1})

	Dy1	Dy2	Dy3	Dy4	Dy5	Dy6
	0.000	0.000	0.000	0.000	0.000	0.000
	201.018	57.496	166.564	175.466	60.539	171.187

	341.003	102.427	269.256	254.437	130.416	256.839
	433.884	153.833	339.928	298.752	229.432	315.947
	519.180	214.356	415.884	359.991	319.494	385.530
	662.761	247.055	547.323	400.416	405.506	425.160
	751.974	270.591	583.759	498.355	479.173	493.242
	806.521	588.670	687.668	754.513	641.985	759.792
	3644.084	3561.607	3627.595	3616.133	3557.947	3614.711
	3807.467	3608.955	3753.272	3735.064	3632.996	3737.814
	3912.218	3659.584	3835.211	3827.852	3742.399	3835.192
	4001.207	3706.336	3913.517	3862.549	3830.880	3885.702
	4089.012	3749.935	3982.152	3896.985	3907.642	3911.244
	4174.819	3860.709	4045.175	3996.498	3957.184	4003.956
	4296.795	3965.330	4155.956	4143.850	4021.632	4148.872
	6246.295	6082.964	6210.621	6186.669	6089.815	6186.732
	6366.863	6151.432	6306.925	6270.962	6207.699	6278.760
	6453.650	6208.223	6374.784	6352.354	6316.226	6367.287
	6539.638	6237.992	6445.809	6386.585	6402.155	6400.891
	6613.488	6374.723	6495.772	6481.490	6447.233	6490.914
	6799.236	6415.497	6663.446	6615.546	6465.784	6620.855
	8244.423	8044.718	8192.542	8162.330	8070.634	8166.539
	8341.615	8116.504	8274.578	8237.131	8199.132	8247.961
	8446.348	8166.286	8364.966	8309.527	8311.973	8324.566
	8515.138	8305.282	8407.917	8399.378	8375.771	8408.615
	8711.928	8338.307	8583.244	8539.189	8392.882	8544.672
	9776.331	9557.424	9715.576	9678.415	9607.108	9687.611
	9902.714	9674.386	9839.460	9796.964	9776.780	9807.754
	10019.745	9777.468	9919.179	9883.155	9881.987	9895.294
	10194.770	9872.547	10082.560	10043.031	9926.850	10051.490
	10209.047	10019.849	10124.057	10119.250	10082.770	10126.135
	10313.232	10033.692	10231.542	10159.224	10088.726	10169.580
	10343.193	10046.079	10256.833	10224.858	10133.918	10229.212
	10394.159	10088.888	10296.546	10261.741	10149.487	10267.758
	10433.981	10131.279	10321.238	10304.932	10192.586	10312.869
	10449.030	10198.701	10346.822	10340.104	10317.383	10351.103
	10902.347	10740.706	10851.986	10838.963	10765.004	10842.117
	11208.703	10846.937	11105.588	11008.552	10989.883	11029.651
	11397.048	11100.912	11262.741	11254.589	11183.970	11261.503
	11719.020	11439.120	11627.613	11584.694	11518.214	11592.802
	11738.432	11490.844	11656.294	11646.273	11550.863	11653.689
	11769.364	11514.508	11679.556	11666.051	11583.427	11671.598
	11807.490	11540.223	11711.966	11685.055	11620.385	11693.443
	11855.252	11552.862	11750.035	11712.965	11647.651	11722.815
	13663.159	13394.698	13569.395	13533.439	13466.482	13543.215
	13695.130	13431.855	13602.716	13564.938	13498.441	13571.514
	13723.009	13462.273	13632.084	13616.490	13552.297	13626.447
	13767.061	13480.641	13671.488	13640.033	13562.345	13649.427
	15125.932	14868.122	15032.600	14997.799	14936.980	15007.126
	15167.953	14884.806	15076.040	15039.876	14961.516	15048.708
	15184.879	14917.390	15090.015	15066.765	15003.385	15076.362
	16018.732	15745.860	15925.905	15890.344	15828.045	15900.512
	16031.937	15762.564	15937.530	15911.567	15837.429	15920.413
	16561.304	16288.168	16465.068	16434.653	16369.027	16444.314
	24749.035	24529.851	24669.236	24630.274	24589.636	24640.198
	24835.321	24622.986	24749.702	24695.904	24655.319	24706.218
	24914.800	24647.243	24828.834	24785.444	24704.429	24793.239
	24956.685	24668.417	24868.086	24826.429	24761.556	24835.397
	25025.212	24811.883	24945.208	24953.323	24882.225	24960.876
	25237.589	25146.324	25203.680	25183.879	25167.735	25186.510
	25377.429	25156.429	25311.198	25297.481	25183.191	25306.207
	25455.190	25202.374	25379.243	25343.477	25260.721	25365.416
	25519.899	25222.921	25439.353	25391.175	25317.024	25397.248
	25578.382	25266.284	25479.122	25413.282	25370.169	25418.953

	25613.534	25299.609	25499.398	25477.871	25441.522	25490.238
	25648.200	25406.826	25543.999	25518.202	25470.194	25527.581
	25719.511	25415.332	25606.530	25606.902	25488.285	25613.134
	27399.842	27216.152	27359.254	27329.837	27224.614	27328.446
	27492.152	27283.645	27422.132	27390.493	27358.465	27402.180
	27575.533	27329.491	27480.346	27439.289	27420.320	27457.434
	27588.316	27361.331	27525.795	27487.648	27469.879	27502.904
	27633.284	27393.006	27530.671	27538.332	27497.902	27548.301
	27711.176	27470.670	27599.812	27583.750	27525.327	27592.187
	27728.418	27537.452	27666.370	27608.052	27586.071	27621.647
	27773.003	27549.990	27682.136	27643.253	27591.090	27657.636
	...	...	...	...	...	...

Table S8. Main values of the *g* tensor of the lowest Kramers doublet on Dy^{3+} sites in complex 1-Dy.

	Dy1	Dy2	Dy3	Dy4	Dy5	Dy6
gx	0.0211	0.0825	0.0437	0.0498	0.0123	0.0390
gy	0.0378	0.1620	0.0886	0.0634	0.0246	0.0527
gz	19.7550	19.7567	19.6271	19.6111	19.5185	19.6850

Table S9. Relative angles between main anisotropy axes on Dy sites in complex 1-Dy.

	Dy1	Dy2	Dy3	Dy4	Dy5	Dy6
Dy1	0.00	22.04	41.66	59.41	40.21	60.13
Dy2	22.04	0.00	20.78	51.60	30.61	51.19
Dy3	41.66	20.78	0.00	58.82	40.98	57.37
Dy4	59.41	51.60	58.82	0.00	21.07	2.64
Dy5	40.21	30.61	40.98	21.07	0.00	20.95
Dy6	60.13	51.19	57.37	2.64	20.95	0.00

Complex 2-Y

In order to estimate the anisotropy of the marginal Mn^{III} ions, fragment ab initio calculations were performed on Mn model fragments.

Computational details

All ab initio calculations were done with MOLCAS 7.4. program package. All basis sets were taken from the ANO-RCC basis set library available in MOLCAS. The following contractions were used for all calculations:

Mn – 7s6p4d3f2g1h.
Y – Y.ECP.Abdalla.0s.0s.0e-AIMP-Cs2NaYCl6.
Zn – Zn.ECP.Lopez-Moraza.0s.0s.0e-AIMP-KZnF3.
N, O – 4s3p2d. (only for the first coordinated atoms, which make a bond with Dy)
C – 4s3p2d. (only for the atoms which are directly bonded to the first coordination sphere of O and N)
N,O, C – 3s2p. (for distant atoms)
H – 2s. (for distant atoms)

Active space of the CASSCF method included 4 electrons in 5 orbitals.
The **spin orbit interaction** was computed by mixing of 5 quintets, 45 triplets and 75 singlet spin free states (all ligand-field states arising from d^4 electronic configuration).

The structure of the calculated Mn^{3+} fragments is listed below.
In all model fragments, neighboring metal ions were modeled by diamagnetic ab initio model potentials available in MOLCAS. Y ions were modeled by Y-AIMP, while the neighboring Mn- by Zn- AIMP.

Structure of the calculated marginal Mn^{3+} fragments

b) b)

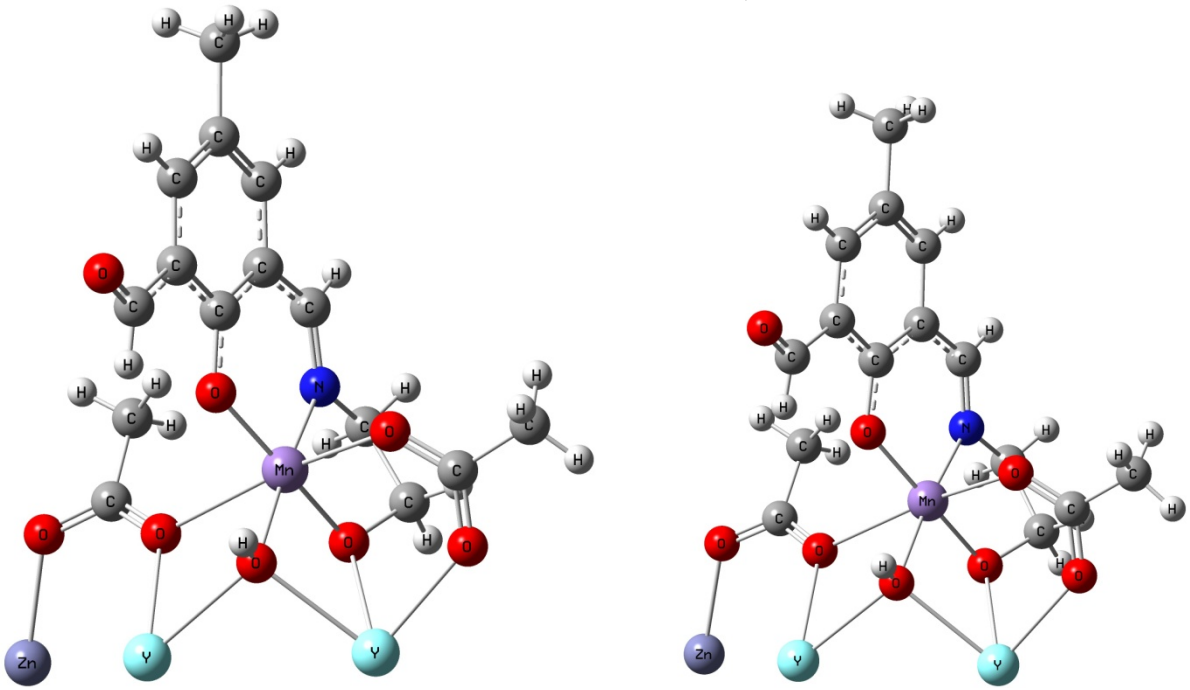

Figure S12. Structure of the calculated marginal Mn13 (left) and marginal Mn14 (right) fragments.

Table S10. Energies of the lowest spin free states of the marginal Mn^{3+} sites.(cm^{-1})

Spin Multiplicity	**Mn13**	**Mn14**
5	0.000	0.000
	16488.700	16744.329
	20104.468	20007.587
	22224.911	22306.065
	24097.761	24287.101
3	17951.095	18002.779
	19194.924	19349.115
	20579.624	20731.248
	22735.750	22722.411
	24352.976	24480.560
	25423.675	25471.647
	26032.857	26165.222
	26599.757	26623.677
	29162.015	29133.988
	33219.820	33145.120
	33835.349	33762.301
	34055.830	34045.881
	36658.292	36621.058
	37487.262	37484.527
	38906.076	39081.590
	39774.230	39744.227
	41543.428	41559.923
	41816.384	41840.271
	42390.190	42309.959
	43429.815	43500.557
	…	…
1	28800.992	28799.651
	29577.626	29630.178
	30353.074	30474.608
	31904.044	31999.041
	31975.958	32097.318

	33985.989	34129.887
	35737.917	35864.219
	36512.921	36518.103
	38204.400	38302.153
	39442.109	39414.534
	41032.938	41111.816
	43767.826	43797.381
	44331.152	44180.403
	45228.244	45141.966
	47860.498	47894.336
	49300.752	49301.794
	49560.350	49545.183
	50047.090	50115.432
	53517.532	53396.350
	54299.041	54260.802
	…	…

Table S11. Energies of the lowest spin-orbit states of the marginal Mn^{3+} sites.(cm^{-1})

	Mn13	**Mn14**
zero field	0.000	0.000
splitting of	0.200	0.190
the ground	7.670	7.717
S=2 state	10.182	10.162
	12.016	12.028
	16424.473	16677.150
	16433.780	16685.725
	16442.303	16696.524
	16475.423	16728.655
	16476.016	16729.553
	17956.595	18011.677
	17963.669	18017.608
	17970.590	18025.672
	19221.416	19373.676
	19225.798	19378.896
	19231.447	19384.283
	20085.734	19992.054
	20086.681	19993.002
	20100.149	20006.210
	20108.707	20014.739
	20111.461	20017.389
	20593.824	20744.844
	20597.568	20748.494
	20604.542	20755.963
	22204.878	22285.726
	22205.225	22286.295
	22218.716	22296.733
	22224.574	22303.665
	22227.678	22305.715
	22738.322	22726.819
	22743.975	22733.130
	22757.150	22746.096
	24054.080	24236.621
	24062.230	24247.262
	24086.723	24273.352
	24112.761	24297.720
	24117.443	24303.958
	24332.107	24461.178
	24372.002	24498.432
	24388.044	24518.846
	…	…

Table S12. Main values of the *g* tensor of the lowest $\tilde{S} = 2$ on Mn^{3+} sites in complex 2-Y.

	Mn13	**Mn14**
gx	1.9722	1.9740
gy	1.9926	1.9925
gz	1.9973	1.9978