Supplementary Information for

A carboxylate based dinuclear dysprosium (III) cluster exhibiting slow magnetic relaxation behaviour

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Table of Contents

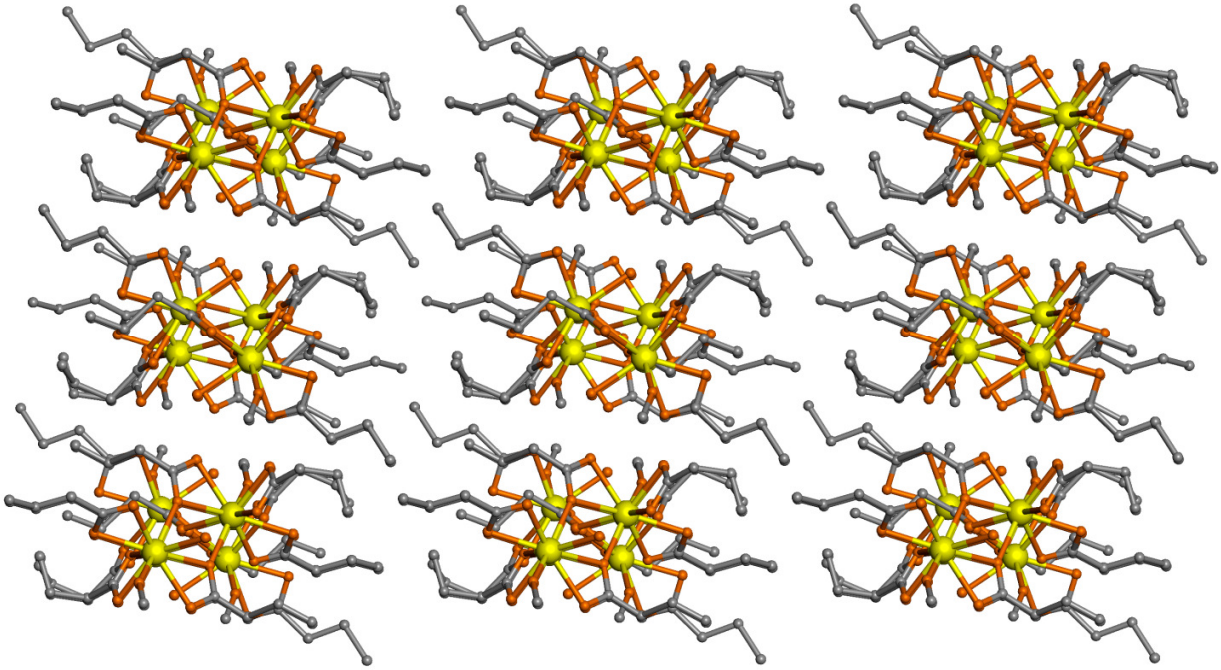

Figure S1. : Molecular packing diagram of compound 1 along ***a*** axis.

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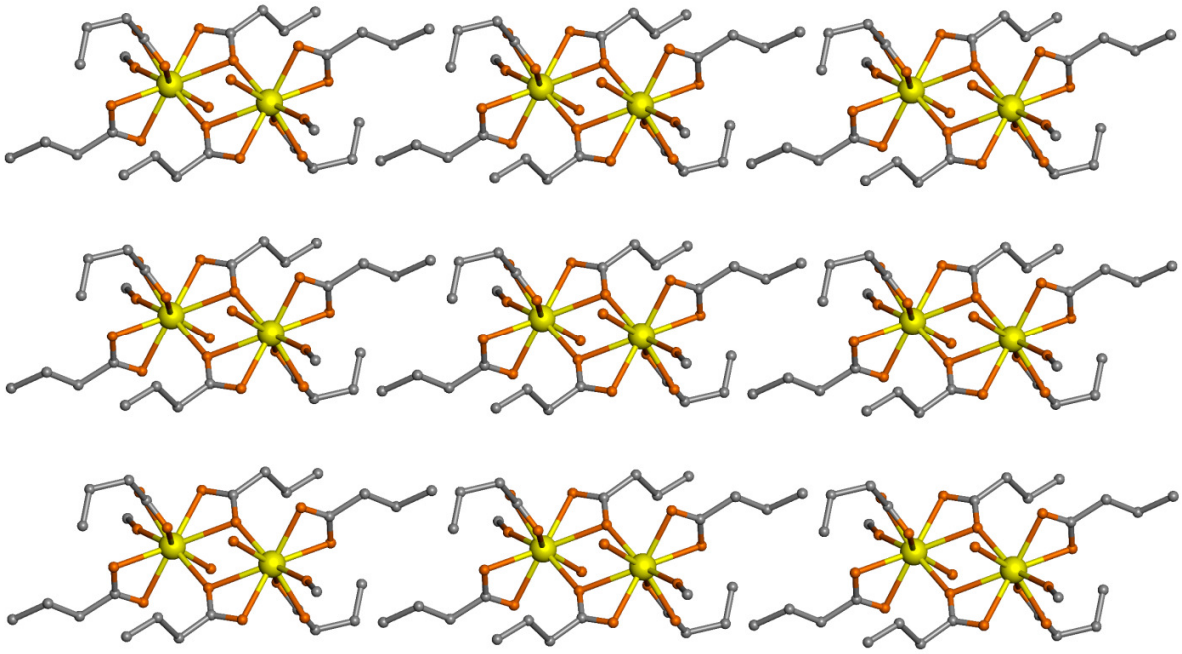

Figure S2. : Molecular packing diagram of compound 1 along ***b*** axis.

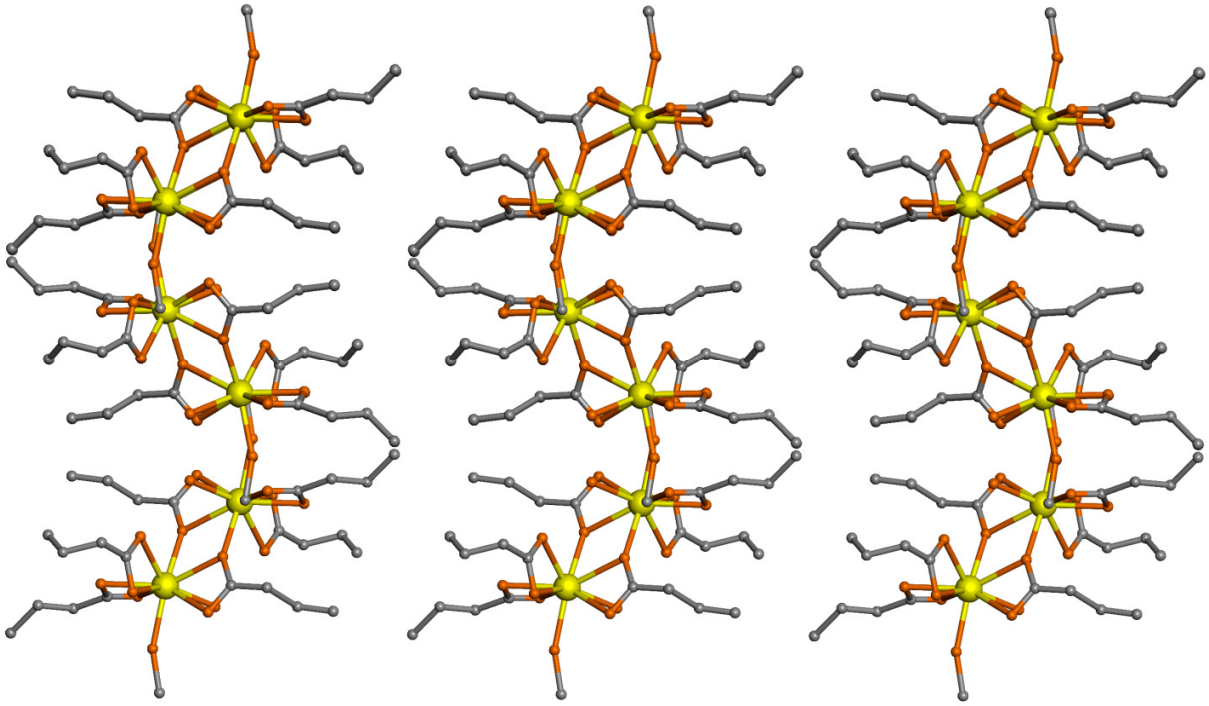

Figure S3. : Molecular packing diagram of compound 1 along ***c*** axis..

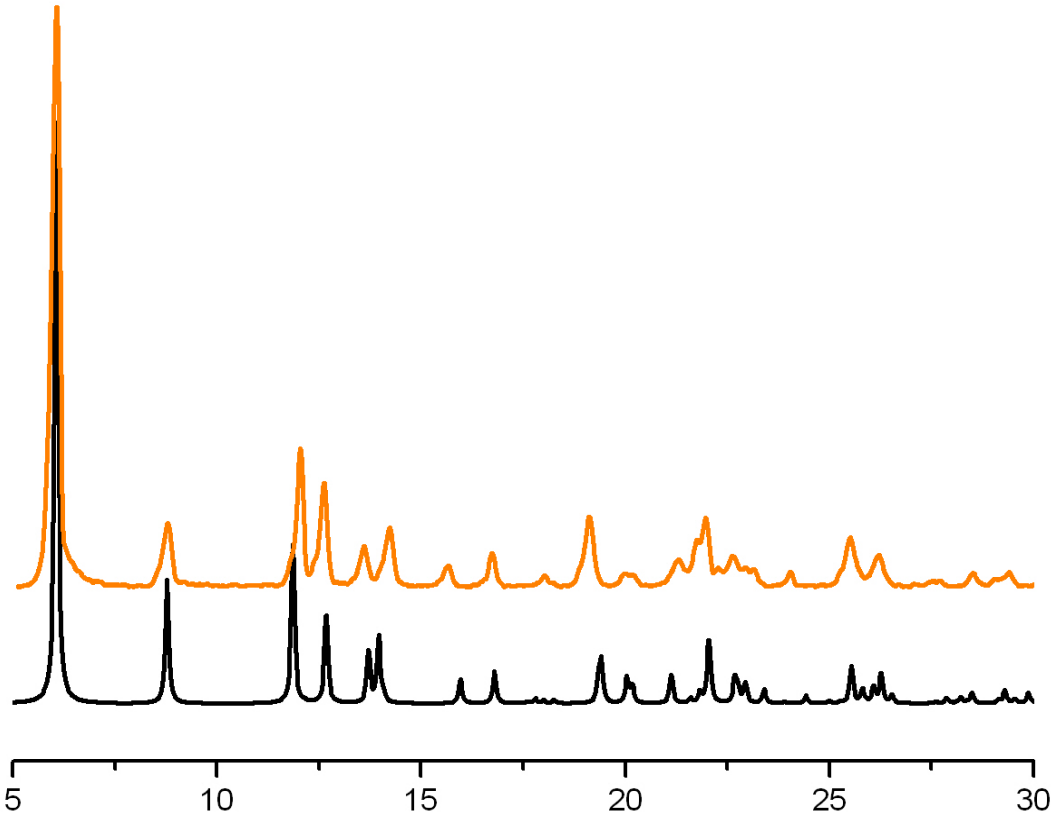

Figure S4: Simulated (Black) and as-synthesized (Orange) powder X- ray diffraction (PXRD) Patterns of compound **1**.

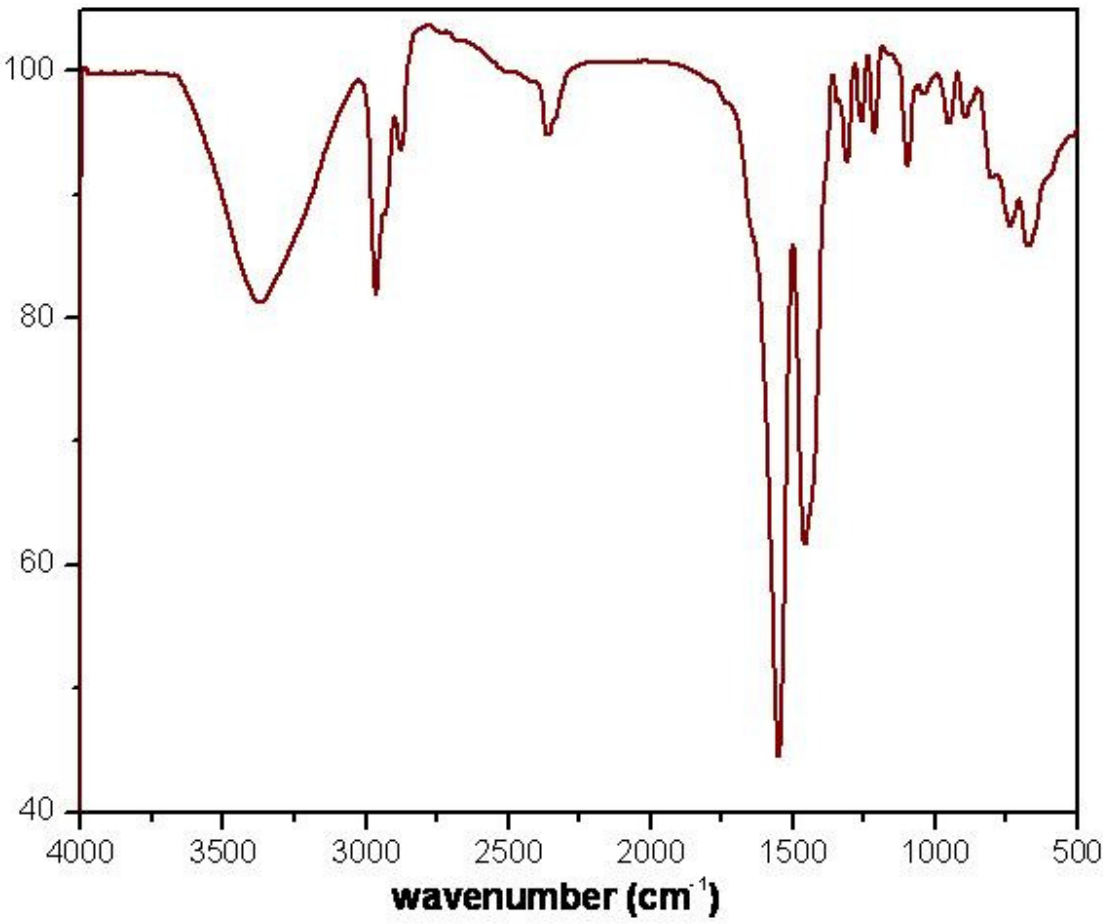

Figure S5. : FT-IR spectra of compound **1**.

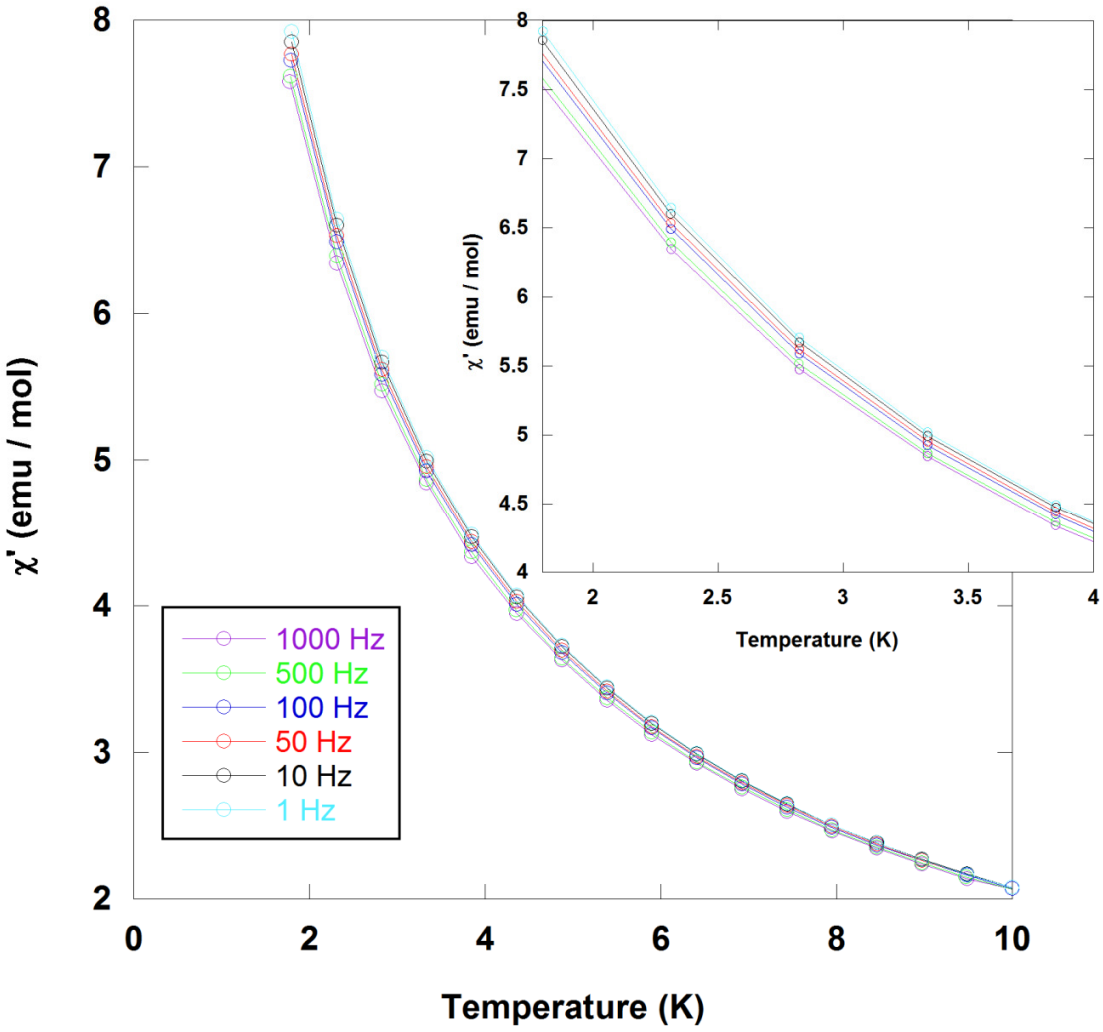

Figure S6: Temperature dependence of the in phase susceptibility for compound **1.**

Table 1. Crystal data and structure refinement for compound **1**.

Identification code	**Compound 1**
Empirical formula	C26 H53 Dy2 O16
Formula weight	946.68
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/C$
Unit cell dimensions	a = 14.710(6) Å
	b = 13.941(6) Å β= 98.046(8) °.
	c = 8.914(4) Å
Volume	1810.0(13) $Å^3$
Z	2
Density (calculated)	1.737 Mg/m^3
Absorption coefficient	4.160 mm^{-1}
F(000)	938
Crystal size	0.12 x 0.10 x 0.09 mm^3
Theta range for data collection	1.40 to 26.24°.
Index ranges	-18<=h<=18, 0<=k<=17, 0<=l<=11
Reflections collected	3659
Independent reflections	3659 [R(int) = 0.0000]
Completeness to theta = 26.24°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7059 and 0.6351
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3659 / 0 / 153
Goodness-of-fit on F^2	1.103
Final R indices [I>2sigma(I)]	R_1 = 0.0242, wR_2 = 0.0650
R indices (all data)	R_1 = 0.0242, wR_2 = 0.0650
Largest diff. peak and hole	1.172 and -0.890 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Compound1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3084(3)	4638(3)	12156(4)	43(1)
C(2)	2496(4)	5000(4)	13228(6)	77(2)
C(3)	1516(7)	4703(9)	12664(13)	149(4)
C(4)	1103(8)	5168(12)	11285(12)	238(10)
C(5)	2630(3)	3627(3)	7609(5)	45(1)
C(6)	1793(3)	3312(4)	6430(6)	66(1)
C(7)	863(8)	3341(10)	7069(15)	160(4)
C(8)	235(11)	2684(12)	6050(17)	220(7)
C(9)	4285(3)	6089(3)	7945(5)	41(1)
C(10)	3399(4)	6155(4)	6944(7)	73(2)
C(11)	2626(8)	6613(9)	7997(13)	150(4)
C(12)	1734(16)	6592(18)	7030(30)	340(12)
C(13)	3916(2)	1121(2)	9558(4)	22(1)
Dy(1)	4076(1)	3903(1)	9832(1)	30(1)
O(1)	3442(2)	5173(2)	11245(3)	47(1)
O(2)	3256(2)	3728(2)	12064(3)	36(1)
O(3)	2458(3)	3968(3)	8909(5)	80(1)
O(4)	3385(2)	3634(2)	7254(3)	35(1)
O(5)	4496(2)	5336(2)	8730(2)	38(1)
O(6)	4846(2)	6774(2)	8093(3)	44(1)
O(7)	3772(2)	2266(2)	9729(3)	47(1)
O(8)	5315(2)	3367(2)	8610(3)	46(1)

Table 3. Bond lengths [Å] and angles [°] for Compound1.

C(1)-O(1)	1.270(5)
C(1)-O(2)	1.299(4)
C(1)-C(2)	1.465(6)
C(1)-Dy(1)	2.885(4)
C(2)-C(3)	1.516(12)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.446(13)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(5)-O(4)	1.197(5)
C(5)-O(3)	1.310(6)
C(5)-C(6)	1.566(7)
C(5)-Dy(1)	2.724(4)
C(6)-C(7)	1.555(12)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-C(8)	1.511(16)
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-O(6)	1.258(5)
C(9)-O(5)	1.276(4)
C(9)-C(10)	1.475(7)
C(9)-Dy(1)#1	2.899(4)
C(10)-C(11)	1.697(12)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(12)	1.46(2)

C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-O(7)	1.621(4)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
Dy(1)-O(7)	2.325(3)
Dy(1)-O(5)	2.346(2)
Dy(1)-O(8)	2.371(3)
Dy(1)-O(3)	2.410(5)
Dy(1)-O(4)	2.409(3)
Dy(1)-O(1)	2.433(3)
Dy(1)-O(6)#1	2.451(3)
Dy(1)-O(2)	2.480(3)
Dy(1)-O(5)#1	2.534(3)
Dy(1)-C(9)#1	2.899(4)
O(5)-Dy(1)#1	2.534(3)
O(6)-Dy(1)#1	2.451(3)

O(1)-C(1)-O(2)	115.5(4)
O(1)-C(1)-C(2)	123.4(4)
O(2)-C(1)-C(2)	121.0(4)
O(1)-C(1)-Dy(1)	56.8(2)
O(2)-C(1)-Dy(1)	59.0(2)
C(2)-C(1)-Dy(1)	174.3(4)
C(1)-C(2)-C(3)	108.1(6)
C(1)-C(2)-H(2A)	110.1
C(3)-C(2)-H(2A)	110.1
C(1)-C(2)-H(2B)	110.1
C(3)-C(2)-H(2B)	110.1
H(2A)-C(2)-H(2B)	108.4
C(4)-C(3)-C(2)	115.3(11)
C(4)-C(3)-H(3A)	108.5

C(2)-C(3)-H(3A)	108.5
C(4)-C(3)-H(3B)	108.5
C(2)-C(3)-H(3B)	108.5
H(3A)-C(3)-H(3B)	107.5
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
O(4)-C(5)-O(3)	122.2(4)
O(4)-C(5)-C(6)	119.7(4)
O(3)-C(5)-C(6)	117.6(4)
O(4)-C(5)-Dy(1)	62.1(2)
O(3)-C(5)-Dy(1)	62.2(3)
C(6)-C(5)-Dy(1)	171.4(3)
C(7)-C(6)-C(5)	113.4(6)
C(7)-C(6)-H(6A)	108.9
C(5)-C(6)-H(6A)	108.9
C(7)-C(6)-H(6B)	108.9
C(5)-C(6)-H(6B)	108.9
H(6A)-C(6)-H(6B)	107.7
C(8)-C(7)-C(6)	105.0(10)
C(8)-C(7)-H(7A)	110.8
C(6)-C(7)-H(7A)	110.8
C(8)-C(7)-H(7B)	110.7
C(6)-C(7)-H(7B)	110.7
H(7A)-C(7)-H(7B)	108.8
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.4
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
O(6)-C(9)-O(5)	117.5(4)
O(6)-C(9)-C(10)	121.8(4)

O(5)-C(9)-C(10)	120.7(4)
O(6)-C(9)-Dy(1)#1	56.93(19)
O(5)-C(9)-Dy(1)#1	60.8(2)
C(10)-C(9)-Dy(1)#1	173.1(3)
C(9)-C(10)-C(11)	107.0(6)
C(9)-C(10)-H(10A)	110.3
C(11)-C(10)-H(10A)	110.3
C(9)-C(10)-H(10B)	110.3
C(11)-C(10)-H(10B)	110.3
H(10A)-C(10)-H(10B)	108.6
C(12)-C(11)-C(10)	106.5(12)
C(12)-C(11)-H(11A)	110.4
C(10)-C(11)-H(11A)	110.4
C(12)-C(11)-H(11B)	110.4
C(10)-C(11)-H(11B)	110.4
H(11A)-C(11)-H(11B)	108.6
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
O(7)-C(13)-H(13A)	109.5
O(7)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
O(7)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
O(7)-Dy(1)-O(5)	151.60(8)
O(7)-Dy(1)-O(8)	80.11(10)
O(5)-Dy(1)-O(8)	79.16(9)
O(7)-Dy(1)-O(3)	81.25(13)
O(5)-Dy(1)-O(3)	97.51(13)
O(8)-Dy(1)-O(3)	129.89(13)
O(7)-Dy(1)-O(4)	75.88(9)
O(5)-Dy(1)-O(4)	80.47(8)

O(8)-Dy(1)-O(4)	76.19(10)
O(3)-Dy(1)-O(4)	54.22(12)
O(7)-Dy(1)-O(1)	130.45(10)
O(5)-Dy(1)-O(1)	74.93(9)
O(8)-Dy(1)-O(1)	147.40(10)
O(3)-Dy(1)-O(1)	73.57(12)
O(4)-Dy(1)-O(1)	117.80(10)
O(7)-Dy(1)-O(6)#1	75.64(10)
O(5)-Dy(1)-O(6)#1	117.63(10)
O(8)-Dy(1)-O(6)#1	76.58(10)
O(3)-Dy(1)-O(6)#1	140.88(13)
O(4)-Dy(1)-O(6)#1	143.33(9)
O(1)-Dy(1)-O(6)#1	98.26(10)
O(7)-Dy(1)-O(2)	79.75(8)
O(5)-Dy(1)-O(2)	127.31(8)
O(8)-Dy(1)-O(2)	146.02(9)
O(3)-Dy(1)-O(2)	73.08(13)
O(4)-Dy(1)-O(2)	124.22(9)
O(1)-Dy(1)-O(2)	52.50(9)
O(6)#1-Dy(1)-O(2)	72.06(10)
O(7)-Dy(1)-O(5)#1	124.88(10)
O(5)-Dy(1)-O(5)#1	66.89(9)
O(8)-Dy(1)-O(5)#1	74.26(10)
O(3)-Dy(1)-O(5)#1	150.01(11)
O(4)-Dy(1)-O(5)#1	139.20(8)
O(1)-Dy(1)-O(5)#1	77.55(10)
O(6)#1-Dy(1)-O(5)#1	51.46(9)
O(2)-Dy(1)-O(5)#1	95.58(9)
O(7)-Dy(1)-C(5)	72.90(12)
O(5)-Dy(1)-C(5)	92.33(11)
O(8)-Dy(1)-C(5)	101.15(12)
O(3)-Dy(1)-C(5)	28.74(13)
O(4)-Dy(1)-C(5)	26.05(11)
O(1)-Dy(1)-C(5)	99.36(12)
O(6)#1-Dy(1)-C(5)	148.35(11)
O(2)-Dy(1)-C(5)	98.71(12)

O(5)#1-Dy(1)-C(5)	159.15(11)
O(7)-Dy(1)-C(1)	105.24(10)
O(5)-Dy(1)-C(1)	100.82(10)
O(8)-Dy(1)-C(1)	160.19(11)
O(3)-Dy(1)-C(1)	69.90(13)
O(4)-Dy(1)-C(1)	123.52(10)
O(1)-Dy(1)-C(1)	25.89(10)
O(6)#1-Dy(1)-C(1)	86.18(11)
O(2)-Dy(1)-C(1)	26.68(9)
O(5)#1-Dy(1)-C(1)	87.43(10)
C(5)-Dy(1)-C(1)	98.65(12)
O(7)-Dy(1)-C(9)#1	99.65(11)
O(5)-Dy(1)-C(9)#1	92.32(10)
O(8)-Dy(1)-C(9)#1	72.32(11)
O(3)-Dy(1)-C(9)#1	157.03(14)
O(4)-Dy(1)-C(9)#1	148.49(10)
O(1)-Dy(1)-C(9)#1	89.17(11)
O(6)#1-Dy(1)-C(9)#1	25.47(10)
O(2)-Dy(1)-C(9)#1	84.44(11)
O(5)#1-Dy(1)-C(9)#1	26.06(9)
C(5)-Dy(1)-C(9)#1	171.11(12)
C(1)-Dy(1)-C(9)#1	87.92(12)
C(1)-O(1)-Dy(1)	97.3(2)
C(1)-O(2)-Dy(1)	94.3(2)
C(5)-O(3)-Dy(1)	89.1(3)
C(5)-O(4)-Dy(1)	91.8(2)
C(9)-O(5)-Dy(1)	150.7(3)
C(9)-O(5)-Dy(1)#1	93.1(2)
Dy(1)-O(5)-Dy(1)#1	113.11(9)
C(9)-O(6)-Dy(1)#1	97.6(2)
C(13)-O(7)-Dy(1)	160.7(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Compound1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	55(2)	33(2)	37(2)	8(2)	-2(2)	4(2)
C(2)	122(5)	60(3)	59(3)	13(3)	52(3)	12(3)
C(4)	215(12)	400(20)	122(8)	91(11)	93(8)	217(15)
Dy(1)	70(1)	11(1)	12(1)	-1(1)	10(1)	-2(1)
O(1)	68(2)	42(2)	35(1)	3(1)	16(1)	1(1)
O(2)	72(2)	20(1)	16(1)	4(1)	11(1)	4(1)
O(3)	89(3)	77(3)	80(3)	-23(2)	28(2)	-7(2)
O(4)	57(2)	28(1)	20(1)	-5(1)	8(1)	-5(1)
O(5)	86(2)	15(1)	13(1)	5(1)	7(1)	-1(1)
O(6)	66(2)	31(1)	33(1)	1(1)	-5(1)	3(1)
O(7)	104(2)	17(1)	25(1)	-4(1)	24(1)	-15(1)
O(8)	76(2)	21(1)	44(2)	-4(1)	20(1)	3(1)