Unusual zig-zag-shape Ln-radical coordination networks derived from a nitronyl nitroxide with two imidazole groups: single-crystal to single-crystal transformations and magnetic properties

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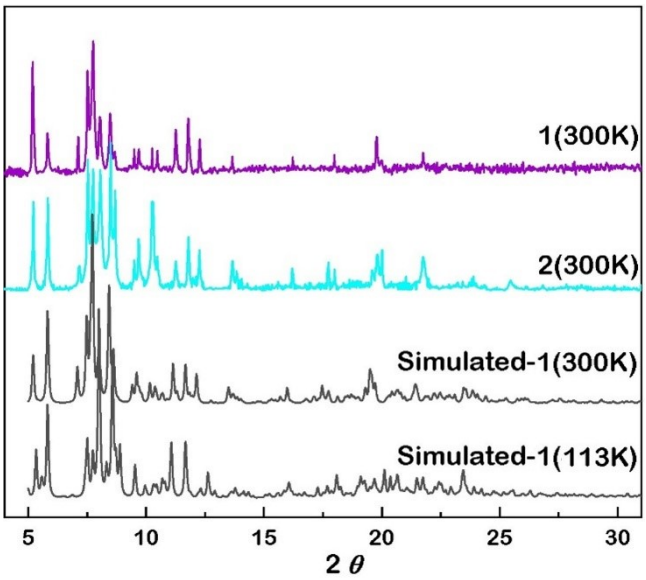

Fig. S1 Powder X-ray diffraction patterns of complexes **1** and **2.**

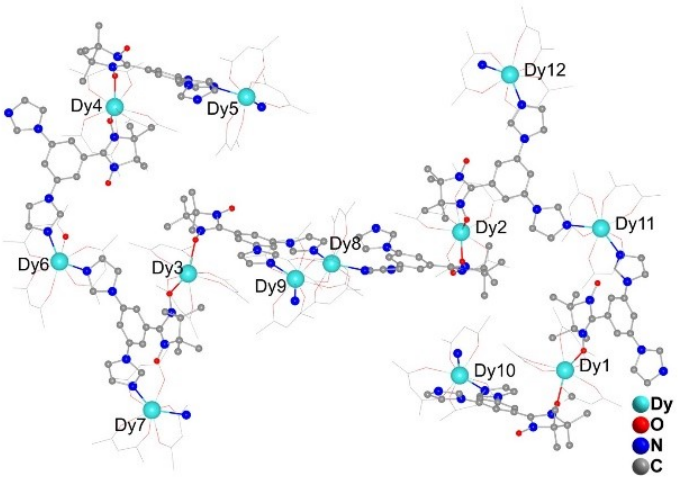

Fig. S2 The asymmetric unit of **2(113K)** (F and H atoms are neglected).

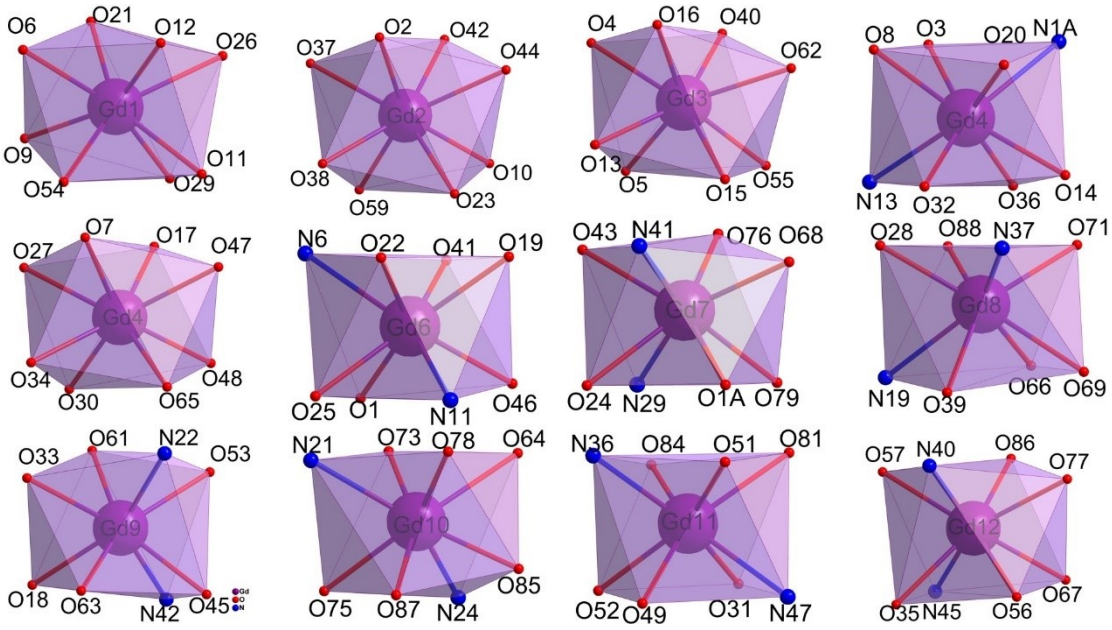

Fig. S3 Coordination polyhedrons of Gd1-Gd12 in **1(113K)**.

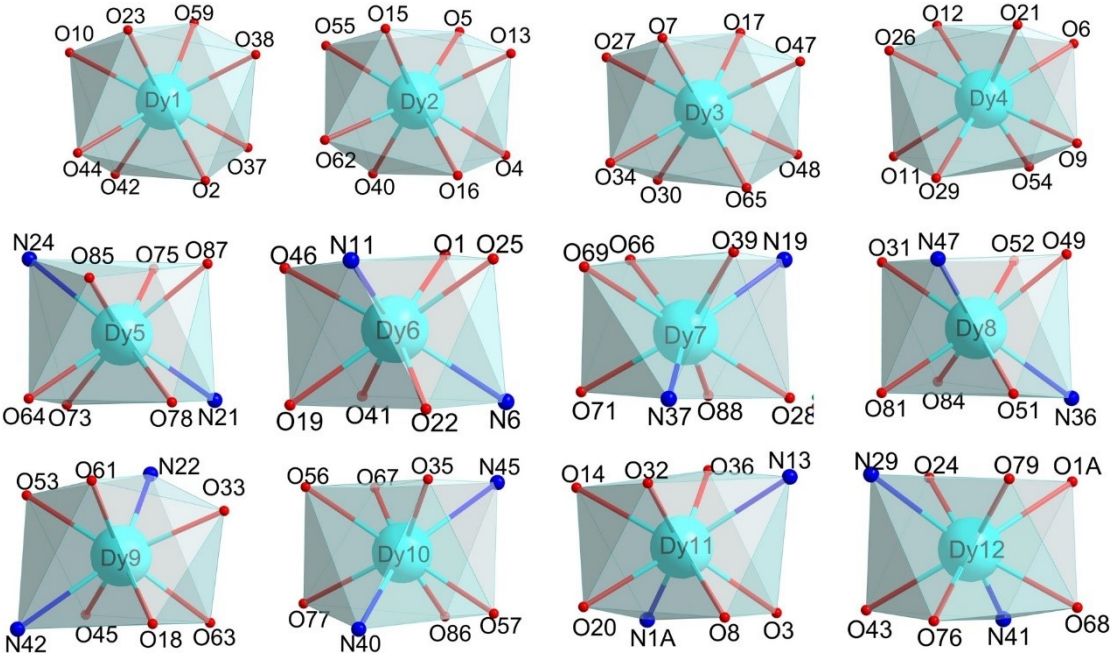

Fig. S4 Coordination polyhedrons of Dy1-Dy12 in **2(113K)**.

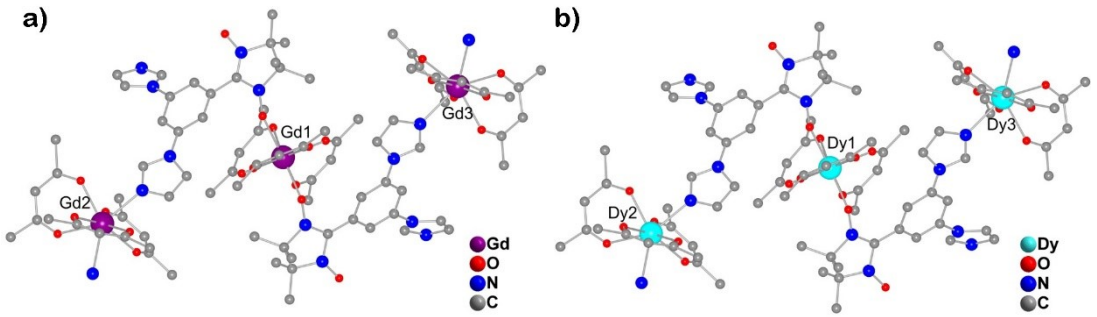

Fig. S5 The asymmetric unit of **1(300K)** a) and **2(300K)** b). (F and H atoms are neglected)

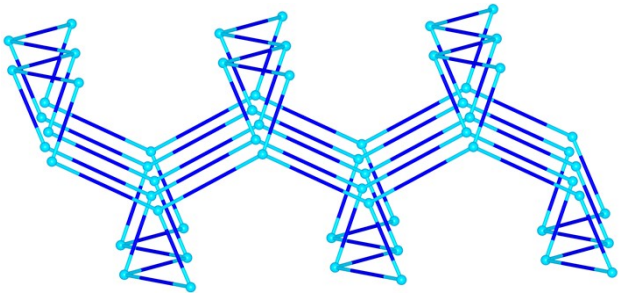

Fig. S6 Topological representation of the 2D network in **2** from the view of *c* axis.

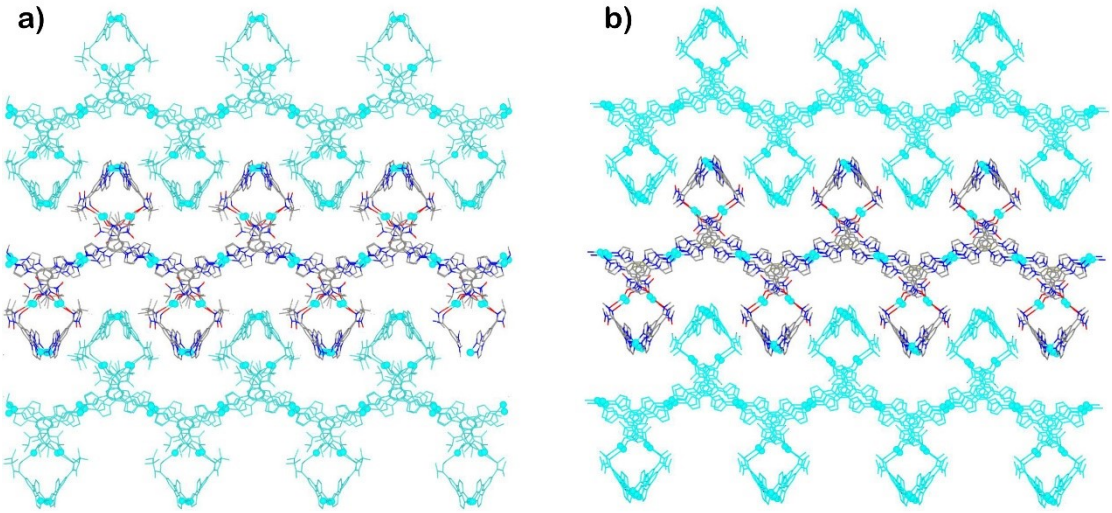

Fig. S7 Side-view of packing patterns of 2D networks of **2** under 113K a) and 300K b). (H, F and hfac co-ligands are omitted)

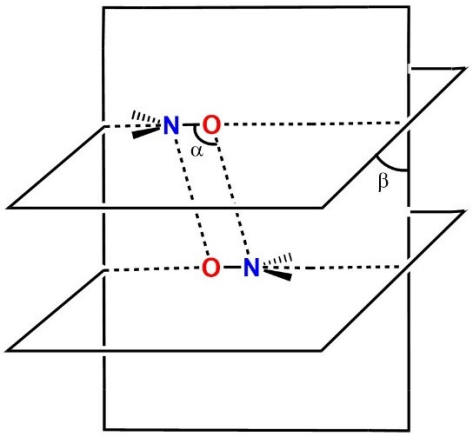

Fig. S8 Definition of the parameters utilized to describe the interaction between two nitroxide groups.

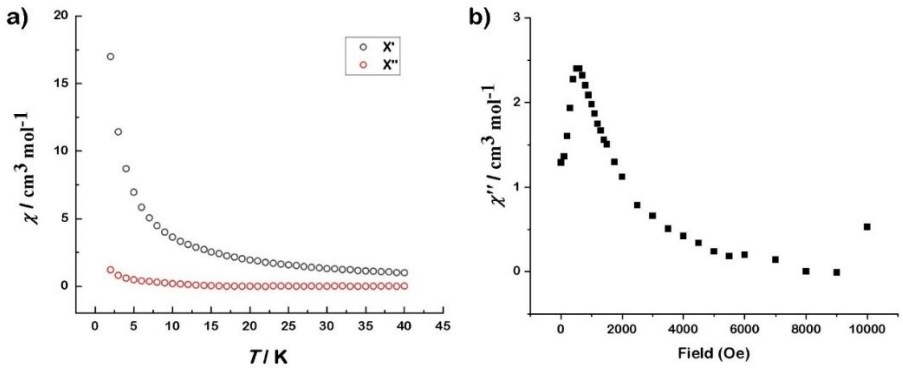

Fig. S9 a) Temperature dependences of χ' and χ'' signals for **2** with zero dc field in an oscillation of 3 Oe at 997Hz. b)The field dependence of χ'' signals of **2** at 1.9 K, 997 Hz.

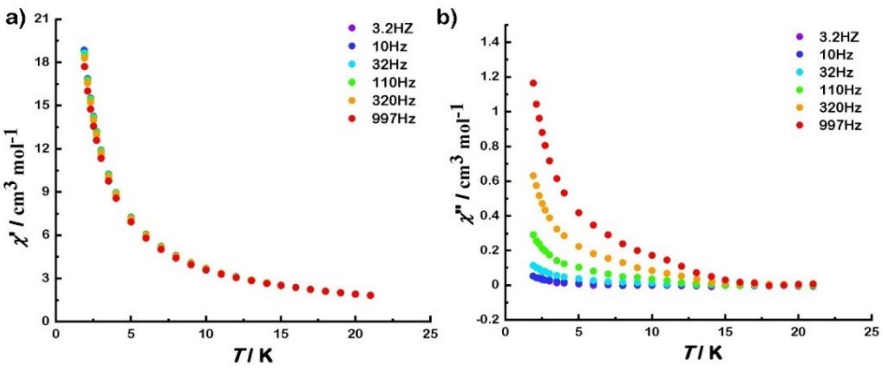

Fig. S10 Temperature dependences of χ' and $\chi''$for **2** in 500Oe dc field with an oscillation of 3 Oe.

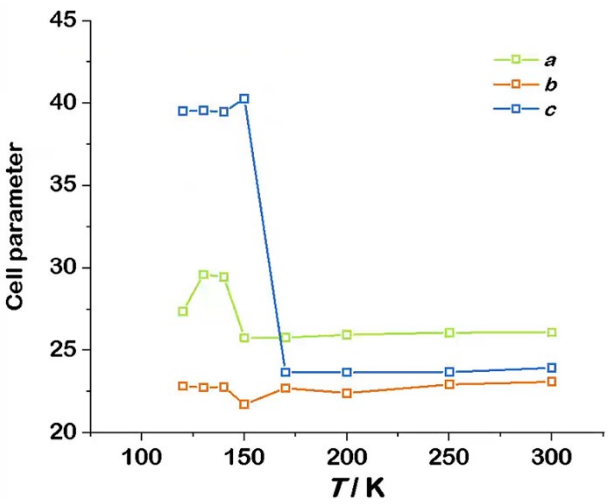

Fig. S11 Plot of the cell parameters vs temperatures of **1**.

Table S1. Selected bond distances (Å) and angles (°) for compound **1(113K)**.

Bond distances			
Gd(1)-O(6)	2.384(17)	Gd(8)-O(28)	2.37(2)
Gd(1)-O(9)	2.36(2)	Gd(8)-O(39)	2.42(2)
Gd(1)-O(11)	2.474(19)	Gd(8)-O(66)	2.40(2)
Gd(1)-O(12)	2.381(17)	Gd(8)-O(69)	2.45(2)
Gd(1)-O(21)	2.38(2)	Gd(8)-O(71)	2.28(2)
Gd(1)-O(26)	2.512(18)	Gd(8)-N(19)	2.531(12)
Gd(1)-O(29)	2.352(16)	Gd(8)-O(88)	2.29(2)
Gd(1)-O(54)	2.326(17)	Gd(8)-N(37)#2	2.404(11)
Gd(2)-O(2)	2.417(17)	Gd(9)-O(18)	2.357(19)
Gd(2)-O(10)	2.437(19)	Gd(9)-O(33)	2.33(2)
Gd(2)-O(23)	2.388(19)	Gd(9)-O(45)	2.35(2)
Gd(2)-O(37)	2.312(18)	Gd(9)-O(53)	2.39(2)
Gd(2)-O(38)	2.341(15)	Gd(9)-O(61)	2.33(2)
Gd(2)-O(42)	2.342(17)	Gd(9)-O(63)	2.30(2)
Gd(2)-O(44)	2.480(16)	Gd(9)-N(42)#3	2.543(12)
Gd(2)-O(59)	2.290(18)	Gd(9)-N(22)	2.422(13)
Gd(3)-O(4)	2.350(17)	Gd(10)-N(21)#1	2.427(14)
Gd(3)-O(5)	2.360(16)	Gd(10)-O(75)	2.30(2)
Gd(3)-O(13)	2.349(18)	Gd(10)-O(78)	2.33(2)
Gd(3)-O(15)	2.422(15)	Gd(10)-O(85)	2.33(3)
Gd(3)-O(16)	2.352(17)	Gd(10)-N(24)	2.481(14)
Gd(3)-O(40)	2.33(2)	Gd(10)-O(87)	2.32(3)
Gd(3)-O(55)	2.408(16)	Gd(10)-O(64A)	2.45(3)
Gd(3)-O(62)	2.451(17)	Gd(10)-O(73A)	2.37(3)
Gd(4)-O(3)	2.364(18)	Gd(11)-O(31)	2.32(2)
Gd(4)-O(8)	2.37(2)	Gd(11)-O(49)	2.40(2)
Gd(4)-O(14)	2.368(18)	Gd(11)-O(51)	2.44(2)
Gd(4)-O(20)	2.36(2)	Gd(11)-O(52)	2.33(2)
Gd(4)-O(32)	2.297(19)	Gd(11)-N(36)	2.384(13)
Gd(4)-O(36)	2.345(19)	Gd(11)-O(81)	2.39(2)
Gd(4)-N(13)	2.48(2)	Gd(11)-O(84)	2.30(2)
Gd(4)-N(1A)	2.479(11)	Gd(11)-N(47)	2.515(15)
Gd(5)-O(7)	2.380(18)	Gd(12)-O(35)	2.35(2)
Gd(5)-O(17)	2.36(2)	Gd(12)-O(56)	2.43(3)
Gd(5)-O(27)	2.39(2)	Gd(12)-O(57)	2.30(2)
Gd(5)-O(30)	2.29(2)	Gd(12)-O(67)	2.33(2)
Gd(5)-O(34)	2.352(18)	Gd(12)-O(77)	2.48(2)
Gd(5)-O(47)	2.415(19)	Gd(12)-O(86)	2.32(2)
Gd(5)-O(48)	2.45(2)	Gd(12)-N(40)	2.503(14)
Gd(5)-O(65)	2.329(19)	Gd(12)-N(45)#4	2.392(13)
Gd(6)-O(1)	2.43(2)	O(2)-N(9)	1.34(3)
Gd(6)-O(19)	2.37(2)	O(15)-N(15)	1.29(3)
Gd(6)-O(22)	2.328(19)	O(17)-N(4)	1.35(3)
Gd(6)-O(25)	2.363(19)	O(21)-N(17)	1.33(3)
Gd(6)-O(41)	2.320(18)	N(32)-O(70)	1.31(3)

Gd(6)-O(46)	2.354(19)	N(12)-O(60)	1.19(3)
Gd(6)-N(6)	2.433(11)	O(40)-N(25)	1.28(3)
Gd(6)-N(11)	2.485(12)	O(54)-N(46)	1.29(3)
Gd(7)-O(24)	2.434(18)	N(20)-O(72)	1.28(3)
Gd(7)-O(43)	2.364(19)	O(58)-N(26)	1.26(3)
Gd(7)-O(1A)	2.475(18)	O(59)-N(33)	1.34(3)
Gd(7)-N(29)	2.496(12)	O(65)-N(44)	1.34(3)
Gd(7)-O(68)	2.32(2)	N(31)-O(74)	1.21(3)
Gd(7)-N(41)#1	2.43(8)	N(34)-O(80)	1.26(3)
Gd(7)-O(76)	2.349(18)	O(82)-N(43)	1.30(3)
Angles			
O(37)-Gd(2)-O(23)	148.8(5)	O(66)-Gd(8)-N(37)#2	145.7(6)
O(37)-Gd(2)-O(44)	130.0(6)	O(71)-Gd(8)-O(28)	120.2(7)
O(38)-Gd(2)-O(2)	76.7(5)	O(71)-Gd(8)-O(39)	137.5(6)
O(38)-Gd(2)-O(10)	130.0(5)	O(71)-Gd(8)-O(66)	74.5(7)
O(38)-Gd(2)-O(23)	73.8(5)	O(71)-Gd(8)-O(69)	72.9(7)
O(38)-Gd(2)-O(37)	75.0(5)	O(71)-Gd(8)-N(19)	142.7(6)
O(38)-Gd(2)-O(44)	128.0(5)	O(71)-Gd(8)-O(88)	77.3(7)
O(42)-Gd(2)-O(2)	93.2(5)	O(71)-Gd(8)-N(37)#2	80.8(6)
O(42)-Gd(2)-O(10)	71.3(5)	N(19)-Gd(8)-O(69)	115.1(6)
O(42)-Gd(2)-O(23)	133.7(5)	O(88)-Gd(8)-O(28)	74.5(7)
O(42)-Gd(2)-O(37)	77.5(5)	O(88)-Gd(8)-O(39)	144.8(7)
O(42)-Gd(2)-O(38)	152.3(5)	O(88)-Gd(8)-O(66)	74.5(7)
O(42)-Gd(2)-O(44)	70.3(4)	O(88)-Gd(8)-O(69)	140.5(7)
O(59)-Gd(2)-O(2)	142.5(5)	O(88)-Gd(8)-N(19)	75.7(6)
O(59)-Gd(2)-O(10)	72.3(5)	O(88)-Gd(8)-N(37)#2	122.8(7)
O(59)-Gd(2)-O(23)	95.2(5)	N(37)#2-Gd(8)-O(39)	77.2(6)
O(59)-Gd(2)-O(37)	76.6(6)	N(37)#2-Gd(8)-O(69)	77.4(6)
O(59)-Gd(2)-O(38)	74.4(6)	N(37)#2-Gd(8)-N(19)	135.9(5)
O(59)-Gd(2)-O(42)	101.3(5)	O(18)-Gd(9)-O(45)	115.5(7)
O(59)-Gd(2)-O(44)	145.8(5)	O(18)-Gd(9)-N(42)#3	72.3(5)
O(4)-Gd(3)-O(15)	146.3(5)	O(18)-Gd(9)-N(22)	151.3(5)
O(4)-Gd(3)-O(55)	132.1(5)	O(33)-Gd(9)-O(18)	74.8(6)
O(4)-Gd(3)-O(62)	132.5(6)	O(33)-Gd(9)-O(45)	136.9(6)
O(5)-Gd(3)-O(4)	72.3(5)	O(33)-Gd(9)-O(53)	125.0(7)
O(5)-Gd(3)-O(13)	74.3(5)	O(33)-Gd(9)-O(61)	75.9(7)
O(5)-Gd(3)-O(15)	102.6(5)	O(33)-Gd(9)-N(42)#3	145.2(6)
O(5)-Gd(3)-O(16)	136.4(5)	O(33)-Gd(9)-N(22)	77.3(6)
O(5)-Gd(3)-O(55)	74.8(5)	O(45)-Gd(9)-N(42)#3	69.9(5)
O(5)-Gd(3)-O(62)	146.5(5)	O(45)-Gd(9)-N(22)	80.9(6)
O(13)-Gd(3)-O(4)	75.5(5)	O(53)-Gd(9)-O(18)	132.0(6)
O(13)-Gd(3)-O(15)	71.2(4)	O(53)-Gd(9)-O(45)	80.9(6)
O(13)-Gd(3)-O(55)	126.6(5)	O(53)-Gd(9)-N(42)#3	72.5(6)
O(13)-Gd(3)-O(62)	128.0(6)	O(53)-Gd(9)-N(22)	71.4(5)
O(15)-Gd(3)-O(62)	69.2(6)	O(61)-Gd(9)-O(18)	81.7(7)
O(16)-Gd(3)-O(4)	72.8(5)	O(61)-Gd(9)-O(45)	144.6(6)
O(16)-Gd(3)-O(13)	72.3(5)	O(61)-Gd(9)-O(53)	65.6(7)
O(16)-Gd(3)-O(15)	92.3(5)	O(61)-Gd(9)-N(42)#3	88.3(6)
O(16)-Gd(3)-O(55)	148.7(5)	O(61)-Gd(9)-N(22)	98.3(6)

O(16)-Gd(3)-O(62)	77.0(5)	O(63)-Gd(9)-O(18)	76.6(6)
O(40)-Gd(3)-O(4)	73.7(6)	O(63)-Gd(9)-O(33)	71.3(7)
O(40)-Gd(3)-O(5)	94.0(5)	O(63)-Gd(9)-O(45)	71.1(6)
O(40)-Gd(3)-O(13)	149.1(5)	O(63)-Gd(9)-O(53)	147.6(6)
O(40)-Gd(3)-O(15)	139.7(5)	O(63)-Gd(9)-O(61)	144.3(7)
O(40)-Gd(3)-O(16)	100.4(5)	O(63)-Gd(9)-N(42)#3	111.1(6)
O(40)-Gd(3)-O(55)	75.0(6)	O(63)-Gd(9)-N(22)	87.9(5)
O(40)-Gd(3)-O(62)	76.7(6)	N(22)-Gd(9)-N(42)#3	136.4(5)
O(55)-Gd(3)-O(15)	74.5(5)	N(21)#1-Gd(10)-O(64)	118.7(6)
O(55)-Gd(3)-O(62)	71.7(5)	N(21)#1-Gd(10)-N(24)	138.7(5)
O(3)-Gd(4)-O(14)	142.2(4)	O(64)-Gd(10)-N(24)	80.6(7)
O(3)-Gd(4)-O(20)	117.1(5)	O(73)-Gd(10)-N(21)#1	75.5(6)
O(3)-Gd(4)-N(13)	75.8(5)	O(73)-Gd(10)-O(64)	68.8(7)
O(3)-Gd(4)-N(1A)	68.7(4)	O(73)-Gd(10)-O(78)	111.1(7)
O(8)-Gd(4)-O(3)	69.6(5)	O(73)-Gd(10)-N(24)	79.5(6)
O(8)-Gd(4)-O(14)	140.8(5)	O(75)-Gd(10)-N(21)#1	74.5(6)
O(8)-Gd(4)-O(20)	74.4(6)	O(75)-Gd(10)-O(64)	143.4(7)
O(8)-Gd(4)-O(36)	147.3(5)	O(75)-Gd(10)-O(73)	83.9(7)
O(8)-Gd(4)-N(13)	80.8(5)	O(75)-Gd(10)-O(78)	140.4(6)
O(8)-Gd(4)-N(1A)	108.8(5)	O(75)-Gd(10)-N(24)	70.5(5)
O(14)-Gd(4)-N(13)	122.0(5)	O(78)-Gd(10)-N(21)#1	74.4(6)
O(14)-Gd(4)-N(1A)	77.9(4)	O(78)-Gd(10)-O(64)	74.4(7)
O(20)-Gd(4)-O(14)	69.6(5)	O(78)-Gd(10)-N(24)	146.2(6)
O(20)-Gd(4)-N(13)	144.5(5)	O(85)-Gd(10)-N(21)#1	144.1(6)
O(20)-Gd(4)-N(1A)	76.8(5)	O(85)-Gd(10)-O(64)	68.8(7)
O(32)-Gd(4)-O(3)	141.4(5)	O(85)-Gd(10)-O(73)	133.4(7)
O(32)-Gd(4)-O(8)	80.1(6)	O(85)-Gd(10)-O(75)	122.1(7)
O(32)-Gd(4)-O(14)	76.0(5)	O(85)-Gd(10)-O(78)	74.6(7)
O(32)-Gd(4)-O(20)	74.9(6)	O(85)-Gd(10)-N(24)	75.3(6)
O(32)-Gd(4)-O(36)	110.7(6)	O(87)-Gd(10)-N(21)#1	87.3(8)
O(32)-Gd(4)-N(13)	76.2(6)	O(87)-Gd(10)-O(64)	134.0(9)
O(32)-Gd(4)-N(1A)	146.7(5)	O(87)-Gd(10)-O(73)	156.9(9)
O(36)-Gd(4)-O(3)	85.4(5)	O(87)-Gd(10)-O(75)	76.7(9)
O(36)-Gd(4)-O(14)	71.4(5)	O(87)-Gd(10)-O(78)	77.9(9)
O(36)-Gd(4)-O(20)	137.7(5)	O(87)-Gd(10)-O(85)	68.8(9)
O(36)-Gd(4)-N(13)	72.6(5)	O(87)-Gd(10)-N(24)	105.0(8)
O(36)-Gd(4)-N(1A)	79.6(5)	O(31)-Gd(11)-O(49)	110.9(7)
N(1A)-Gd(4)-N(13)	136.2(5)	O(31)-Gd(11)-O(51)	138.9(6)
O(7)-Gd(5)-O(17)	98.1(5)	O(31)-Gd(11)-N(36)	148.6(6)
O(7)-Gd(5)-O(27)	73.1(5)	O(31)-Gd(11)-O(81)	77.5(7)
O(7)-Gd(5)-O(34)	74.0(5)	O(31)-Gd(11)-N(47)	73.9(6)
O(7)-Gd(5)-O(47)	75.0(5)	O(49)-Gd(11)-O(51)	82.3(6)
O(7)-Gd(5)-O(48)	146.0(5)	O(49)-Gd(11)-N(36)	80.0(6)
O(17)-Gd(5)-O(27)	72.1(5)	O(49)-Gd(11)-O(81)	142.7(7)
O(17)-Gd(5)-O(47)	74.9(6)	O(49)-Gd(11)-N(47)	70.6(6)
O(17)-Gd(5)-O(48)	68.8(6)	O(51)-Gd(11)-N(47)	74.6(6)
O(27)-Gd(5)-O(47)	129.5(5)	O(52)-Gd(11)-O(31)	73.8(6)
O(27)-Gd(5)-O(48)	126.9(5)	O(52)-Gd(11)-O(49)	69.4(6)
O(30)-Gd(5)-O(7)	135.3(5)	O(52)-Gd(11)-O(51)	144.3(6)

O(30)-Gd(5)-O(17)	94.0(5)	O(52)-Gd(11)-N(36)	83.6(6)
O(30)-Gd(5)-O(27)	70.1(5)	O(52)-Gd(11)-O(81)	144.1(7)
O(30)-Gd(5)-O(34)	72.3(6)	O(52)-Gd(11)-O(84)	73.2(6)
O(30)-Gd(5)-O(47)	149.5(5)	O(52)-Gd(11)-N(47)	113.6(6)
O(30)-Gd(5)-O(48)	78.2(5)	N(36)-Gd(11)-O(51)	70.1(6)
O(30)-Gd(5)-O(65)	101.9(6)	N(36)-Gd(11)-O(81)	112.3(7)
O(34)-Gd(5)-O(17)	146.2(6)	N(36)-Gd(11)-N(47)	136.4(5)
O(34)-Gd(5)-O(27)	74.1(5)	O(81)-Gd(11)-O(51)	70.5(6)
O(34)-Gd(5)-O(47)	131.2(6)	O(81)-Gd(11)-N(47)	77.7(8)
O(34)-Gd(5)-O(48)	133.9(6)	O(84)-Gd(11)-O(31)	73.6(7)
O(47)-Gd(5)-O(48)	71.4(5)	O(84)-Gd(11)-O(49)	138.8(6)
O(65)-Gd(5)-O(7)	97.3(5)	O(84)-Gd(11)-O(51)	122.4(7)
O(65)-Gd(5)-O(17)	137.9(6)	O(84)-Gd(11)-N(36)	79.2(6)
O(65)-Gd(5)-O(27)	150.0(5)	O(84)-Gd(11)-O(81)	78.4(7)
O(65)-Gd(5)-O(34)	75.9(6)	O(84)-Gd(11)-N(47)	143.0(6)
O(65)-Gd(5)-O(47)	71.8(6)	O(35)-Gd(12)-O(56)	68.3(7)
O(65)-Gd(5)-O(48)	76.7(6)	O(35)-Gd(12)-O(77)	133.4(6)
O(1)-Gd(6)-N(6)	79.7(5)	O(35)-Gd(12)-N(40)	81.6(6)
O(1)-Gd(6)-N(11)	112.1(5)	O(35)-Gd(12)-N(45)#4	70.3(5)
O(19)-Gd(6)-O(1)	144.5(6)	O(56)-Gd(12)-N(40)	82.5(6)
O(19)-Gd(6)-O(41)	73.4(5)	O(57)-Gd(12)-O(56)	144.5(7)
O(19)-Gd(6)-N(6)	113.1(5)	O(57)-Gd(12)-O(67)	140.4(6)
O(19)-Gd(6)-N(11)	81.3(5)	O(57)-Gd(12)-O(77)	124.7(7)
O(22)-Gd(6)-O(1)	144.0(5)	O(57)-Gd(12)-N(40)	72.1(6)
O(22)-Gd(6)-O(19)	69.7(5)	O(57)-Gd(12)-N(45)#4	76.5(6)
O(22)-Gd(6)-O(25)	80.5(5)	O(67)-Gd(12)-O(35)	111.1(6)
O(22)-Gd(6)-O(41)	115.1(5)	O(67)-Gd(12)-O(56)	72.6(6)
O(22)-Gd(6)-O(46)	136.9(5)	O(67)-Gd(12)-O(77)	72.2(7)
O(22)-Gd(6)-N(6)	72.9(5)	O(67)-Gd(12)-N(40)	144.2(6)
O(22)-Gd(6)-N(11)	76.3(5)	O(67)-Gd(12)-N(45)#4	74.8(6)
O(25)-Gd(6)-O(1)	71.3(5)	O(77)-Gd(12)-O(56)	69.0(8)
O(25)-Gd(6)-N(6)	78.2(5)	O(77)-Gd(12)-N(40)	75.1(6)
O(25)-Gd(6)-N(11)	68.9(5)	O(86)-Gd(12)-O(35)	149.9(6)
O(41)-Gd(6)-O(25)	142.9(4)	O(86)-Gd(12)-O(57)	74.8(7)
O(41)-Gd(6)-N(6)	75.3(5)	O(86)-Gd(12)-O(67)	75.8(6)
O(41)-Gd(6)-N(11)	145.2(5)	O(86)-Gd(12)-O(77)	76.7(7)
O(46)-Gd(6)-O(1)	77.9(5)	O(86)-Gd(12)-N(40)	110.5(6)
O(46)-Gd(6)-O(19)	73.4(5)	O(86)-Gd(12)-N(45)#4	84.3(6)
O(46)-Gd(6)-O(25)	119.5(6)	N(45)#4-Gd(12)-O(56)	111.5(7)
O(46)-Gd(6)-O(41)	73.2(5)	N(45)#4-Gd(12)-O(77)	145.0(6)
O(46)-Gd(6)-N(6)	144.2(5)	N(45)#4-Gd(12)-N(40)	139.7(5)
O(46)-Gd(6)-N(11)	77.0(5)	N(9)-O(2)-Gd(2)	133.5(11)
N(6)-Gd(6)-N(11)	137.9(5)	N(15)-O(15)-Gd(3)	133.2(10)
O(24)-Gd(7)-O(1A)	69.8(5)	N(4)-O(17)-Gd(5)	134.0(12)
O(24)-Gd(7)-N(29)	70.1(5)	N(17)-O(21)-Gd(1)	141.4(12)

Symmetry transformations used to generate equivalent atoms:

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

Table S2. Selected bond distances (Å) and angles (°) for compound **2(113K)**.

Bond distances			
Dy(1)-O(6)	2.36(2)	Dy(8)-O(28)	2.27(3)
Dy(1)-O(9)	2.31(2)	Dy(8)-O(39)	2.37(2)
Dy(1)-O(11)	2.42(2)	Dy(8)-O(66)	2.30(3)
Dy(1)-O(12)	2.36(2)	Dy(8)-O(69)	2.43(2)
Dy(1)-O(21)	2.35(2)	Dy(8)-O(71)	2.22(3)
Dy(1)-O(26)	2.39(2)	Dy(8)-N(19)	2.431(15)
Dy(1)-O(29)	2.34(2)	Dy(8)-O(88)	2.28(3)
Dy(1)-O(54)	2.34(2)	Dy(8)-N(37)#2	2.382(15)
Dy(2)-O(2)	2.37(2)	Dy(9)-O(18)	2.36(2)
Dy(2)-O(10)	2.41(2)	Dy(9)-O(33)	2.34(3)
Dy(2)-O(23)	2.35(2)	Dy(9)-O(45)	2.31(3)
Dy(2)-O(37)	2.35(2)	Dy(9)-O(53)	2.21(3)
Dy(2)-O(38)	2.32(2)	Dy(9)-O(61)	2.29(2)
Dy(2)-O(42)	2.32(2)	Dy(9)-O(63)	2.31(2)
Dy(2)-O(44)	2.403(19)	Dy(9)-N(42)#3	2.512(16)
Dy(2)-O(59)	2.31(2)	Dy(9)-N(22)	2.401(15)
Dy(3)-O(4)	2.38(2)	Dy(10)-N(21)#1	2.463(16)
Dy(3)-O(5)	2.32(2)	Dy(10)-O(75)	2.35(3)
Dy(3)-O(13)	2.318(18)	Dy(10)-O(78)	2.36(3)
Dy(3)-O(15)	2.34(2)	Dy(10)-O(85)	2.24(3)
Dy(3)-O(16)	2.34(2)	Dy(10)-N(24)	2.391(15)
Dy(3)-O(40)	2.29(3)	Dy(10)-O(87)	2.25(3)
Dy(3)-O(55)	2.33(2)	Dy(10)-O(64A)	2.39(3)
Dy(3)-O(62)	2.35(2)	Dy(10)-O(73A)	2.34(3)
Dy(4)-O(3)	2.31(2)	Dy(11)-O(31)	2.29(2)
Dy(4)-O(8)	2.31(2)	Dy(11)-O(49)	2.32(3)
Dy(4)-O(14)	2.39(2)	Dy(11)-O(51)	2.35(3)
Dy(4)-O(20)	2.31(2)	Dy(11)-O(52)	2.38(3)
Dy(4)-O(32)	2.30(2)	Dy(11)-N(36)	2.359(16)
Dy(4)-O(36)	2.34(2)	Dy(11)-O(81)	2.34(3)
Dy(4)-N(13)	2.46(3)	Dy(11)-O(84)	2.30(3)
Dy(4)-N(1A)	2.415(14)	Dy(11)-N(47)	2.433(19)
Dy(5)-O(7)	2.296(19)	Dy(12)-O(35)	2.40(3)
Dy(5)-O(17)	2.33(2)	Dy(12)-O(56)	2.37(3)
Dy(5)-O(27)	2.37(2)	Dy(12)-O(57)	2.32(3)
Dy(5)-O(30)	2.28(2)	Dy(12)-O(67)	2.32(3)
Dy(5)-O(34)	2.36(2)	Dy(12)-O(77)	2.40(3)
Dy(5)-O(47)	2.38(2)	Dy(12)-O(86)	2.33(3)
Dy(5)-O(48)	2.39(2)	Dy(12)-N(40)	2.451(19)
Dy(5)-O(65)	2.29(2)	Dy(12)-N(45)#4	2.383(18)
Dy(6)-O(1)	2.35(2)	O(2)-N(9)	1.32(3)
Dy(6)-O(19)	2.37(2)	O(15)-N(15)	1.33(3)
Dy(6)-O(22)	2.34(2)	O(17)-N(4)	1.35(3)
Dy(6)-O(25)	2.330(19)	O(21)-N(17)	1.31(3)
Dy(6)-O(41)	2.32(2)	N(32)-O(70)	1.23(4)
Dy(6)-O(46)	2.38(2)	N(12)-O(60)	1.28(3)

Dy(6)-N(6)	2.416(14)	O(40)-N(25)	1.32(4)
Dy(6)-N(11)	2.406(15)	O(54)-N(46)	1.28(3)
Dy(7)-O(24)	2.35(3)	N(20)-O(72)	1.29(4)
Dy(7)-O(43)	2.33(2)	O(58)-N(26)	1.27(4)
Dy(7)-O(1A)	2.412(19)	O(59)-N(33)	1.27(4)
Dy(7)-N(29)	2.432(17)	O(65)-N(44)	1.31(4)
Dy(7)-O(68)	2.30(4)	N(31)-O(74)	1.26(4)
Dy(7)-N(41)#1	2.41(9)	N(34)-O(80)	1.25(4)
Dy(7)-O(76)	2.30(3)	O(82)-N(43)	1.28(4)
Dy(7)-O(79)	2.33(3)	O(83)-N(28)	1.29(4)
Angles			
O(6)-Dy(1)-O(11)	127.2(6)	O(24)-Dy(7)-O(1A)	70.4(7)
O(6)-Dy(1)-O(12)	74.3(6)	O(24)-Dy(7)-N(29)	71.5(7)
O(6)-Dy(1)-O(26)	126.3(6)	O(24)-Dy(7)-N(41)#1	75(10)
O(9)-Dy(1)-O(6)	75.9(6)	O(43)-Dy(7)-O(24)	76.8(7)
O(9)-Dy(1)-O(11)	129.1(6)	O(43)-Dy(7)-O(1A)	140.0(7)
O(9)-Dy(1)-O(12)	150.2(6)	O(43)-Dy(7)-N(29)	75.9(8)
O(9)-Dy(1)-O(21)	71.7(7)	O(43)-Dy(7)-N(41)#1	72(7)
O(9)-Dy(1)-O(26)	128.2(6)	O(43)-Dy(7)-O(79)	139.9(8)
O(9)-Dy(1)-O(29)	78.2(6)	O(1A)-Dy(7)-N(29)	113.1(7)
O(9)-Dy(1)-O(54)	77.8(7)	O(68)-Dy(7)-O(24)	138.9(7)
O(12)-Dy(1)-O(11)	71.6(5)	O(68)-Dy(7)-O(43)	124.8(10)
O(12)-Dy(1)-O(26)	71.9(6)	O(68)-Dy(7)-O(1A)	73.0(8)
O(21)-Dy(1)-O(6)	76.6(6)	O(68)-Dy(7)-N(29)	142.2(8)
O(21)-Dy(1)-O(11)	148.6(6)	O(68)-Dy(7)-N(41)#1	79(8)
O(21)-Dy(1)-O(12)	101.1(6)	O(68)-Dy(7)-O(79)	75.9(11)
O(21)-Dy(1)-O(26)	70.5(6)	N(41)#1-Dy(7)-O(1A)	78(9)
O(26)-Dy(1)-O(11)	78.3(6)	N(41)#1-Dy(7)-N(29)	138(8)
O(29)-Dy(1)-O(6)	153.9(6)	O(76)-Dy(7)-O(24)	144.6(7)
O(29)-Dy(1)-O(11)	69.2(6)	O(76)-Dy(7)-O(43)	74.2(8)
O(29)-Dy(1)-O(12)	131.6(6)	O(76)-Dy(7)-O(1A)	143.8(7)
O(29)-Dy(1)-O(21)	98.0(6)	O(76)-Dy(7)-N(29)	82.0(9)
O(29)-Dy(1)-O(26)	73.4(6)	O(76)-Dy(7)-O(68)	75.7(8)
O(29)-Dy(1)-O(54)	100.0(6)	O(76)-Dy(7)-N(41)#1	113(10)
O(54)-Dy(1)-O(6)	71.8(6)	O(76)-Dy(7)-O(79)	80.1(9)
O(54)-Dy(1)-O(11)	71.0(6)	O(79)-Dy(7)-O(24)	111.2(9)
O(54)-Dy(1)-O(12)	92.9(6)	O(79)-Dy(7)-O(1A)	75.1(7)
O(54)-Dy(1)-O(21)	140.4(6)	O(79)-Dy(7)-N(29)	70.4(8)
O(54)-Dy(1)-O(26)	148.9(6)	O(79)-Dy(7)-N(41)#1	148(7)
O(2)-Dy(2)-O(10)	146.3(6)	O(28)-Dy(8)-O(39)	84.6(7)
O(2)-Dy(2)-O(44)	71.0(6)	O(28)-Dy(8)-O(66)	140.8(8)
O(10)-Dy(2)-O(44)	75.4(6)	O(28)-Dy(8)-O(69)	144.3(7)
O(23)-Dy(2)-O(2)	98.4(6)	O(28)-Dy(8)-N(19)	75.0(7)
O(23)-Dy(2)-O(10)	73.0(6)	O(28)-Dy(8)-O(88)	73.9(9)
O(23)-Dy(2)-O(37)	149.6(7)	O(28)-Dy(8)-N(37)#2	72.2(7)
O(23)-Dy(2)-O(44)	72.1(6)	O(39)-Dy(8)-O(69)	70.0(7)
O(37)-Dy(2)-O(2)	74.8(8)	O(39)-Dy(8)-N(19)	72.3(6)
O(37)-Dy(2)-O(10)	128.2(8)	O(39)-Dy(8)-N(37)#2	75.7(7)
O(37)-Dy(2)-O(44)	129.7(7)	O(66)-Dy(8)-O(39)	108.6(8)

O(38)-Dy(2)-O(2)	75.7(7)	O(66)-Dy(8)-O(69)	73.1(8)
O(38)-Dy(2)-O(10)	129.6(7)	O(66)-Dy(8)-N(19)	74.5(7)
O(38)-Dy(2)-O(23)	74.6(7)	O(66)-Dy(8)-N(37)#2	146.1(7)
O(38)-Dy(2)-O(37)	74.9(7)	O(71)-Dy(8)-O(28)	117.8(9)
O(38)-Dy(2)-O(44)	128.1(8)	O(71)-Dy(8)-O(39)	139.8(8)
O(42)-Dy(2)-O(2)	94.4(6)	O(71)-Dy(8)-O(66)	75.8(9)
O(42)-Dy(2)-O(10)	72.7(6)	O(71)-Dy(8)-O(69)	73.7(9)
O(42)-Dy(2)-O(23)	135.2(6)	O(71)-Dy(8)-N(19)	142.6(8)
O(42)-Dy(2)-O(37)	75.3(6)	O(71)-Dy(8)-O(88)	73.8(9)
O(42)-Dy(2)-O(38)	150.1(6)	O(71)-Dy(8)-N(37)#2	80.2(8)
O(42)-Dy(2)-O(44)	71.9(6)	N(19)-Dy(8)-O(69)	117.7(7)
O(59)-Dy(2)-O(2)	141.3(7)	O(88)-Dy(8)-O(39)	146.4(8)
O(59)-Dy(2)-O(10)	72.4(7)	O(88)-Dy(8)-O(66)	75.9(9)
O(59)-Dy(2)-O(23)	95.7(7)	O(88)-Dy(8)-O(69)	139.4(9)
O(59)-Dy(2)-O(37)	74.8(8)	O(88)-Dy(8)-N(19)	77.3(8)
O(59)-Dy(2)-O(38)	73.6(8)	O(88)-Dy(8)-N(37)#2	119.7(9)
O(59)-Dy(2)-O(42)	100.6(6)	N(37)#2-Dy(8)-O(69)	77.4(7)
O(59)-Dy(2)-O(44)	147.7(7)	N(37)#2-Dy(8)-N(19)	135.7(7)
O(5)-Dy(3)-O(4)	71.9(6)	O(18)-Dy(9)-N(42)#3	73.5(7)
O(5)-Dy(3)-O(13)	71.7(5)	O(18)-Dy(9)-N(22)	150.3(7)
O(5)-Dy(3)-O(15)	102.3(6)	O(33)-Dy(9)-O(18)	74.7(7)
O(5)-Dy(3)-O(16)	135.6(6)	O(33)-Dy(9)-N(42)#3	146.5(7)
O(5)-Dy(3)-O(55)	76.2(6)	O(33)-Dy(9)-N(22)	76.7(7)
O(5)-Dy(3)-O(62)	149.0(7)	O(45)-Dy(9)-O(18)	116.1(8)
O(13)-Dy(3)-O(4)	72.8(6)	O(45)-Dy(9)-O(33)	134.6(8)
O(13)-Dy(3)-O(15)	72.0(6)	O(45)-Dy(9)-N(42)#3	70.8(7)
O(13)-Dy(3)-O(16)	73.3(6)	O(45)-Dy(9)-N(22)	79.4(7)
O(13)-Dy(3)-O(62)	128.4(7)	O(53)-Dy(9)-O(18)	132.7(7)
O(15)-Dy(3)-O(4)	144.2(6)	O(53)-Dy(9)-O(33)	125.3(9)
O(15)-Dy(3)-O(16)	91.8(6)	O(53)-Dy(9)-O(45)	81.4(9)
O(15)-Dy(3)-O(62)	69.2(8)	O(53)-Dy(9)-O(61)	68.2(9)
O(16)-Dy(3)-O(4)	72.3(6)	O(53)-Dy(9)-O(63)	148.6(8)
O(16)-Dy(3)-O(62)	75.4(7)	O(53)-Dy(9)-N(42)#3	72.1(8)
O(40)-Dy(3)-O(4)	74.0(7)	O(53)-Dy(9)-N(22)	72.0(7)
O(40)-Dy(3)-O(5)	95.1(6)	O(61)-Dy(9)-O(18)	80.6(7)
O(40)-Dy(3)-O(13)	146.7(7)	O(61)-Dy(9)-O(33)	74.2(9)
O(40)-Dy(3)-O(15)	141.3(7)	O(61)-Dy(9)-O(45)	148.1(8)
O(40)-Dy(3)-O(16)	99.4(6)	O(61)-Dy(9)-O(63)	141.3(8)
O(40)-Dy(3)-O(55)	76.1(8)	O(61)-Dy(9)-N(42)#3	90.2(8)
O(40)-Dy(3)-O(62)	78.0(8)	O(61)-Dy(9)-N(22)	99.3(7)
O(55)-Dy(3)-O(4)	133.5(6)	O(63)-Dy(9)-O(18)	74.4(7)
O(55)-Dy(3)-O(13)	126.9(7)	O(63)-Dy(9)-O(33)	71.0(8)
O(55)-Dy(3)-O(15)	75.1(7)	O(63)-Dy(9)-O(45)	70.5(8)
O(55)-Dy(3)-O(16)	148.1(6)	O(63)-Dy(9)-N(42)#3	110.0(8)
O(55)-Dy(3)-O(62)	72.8(7)	O(63)-Dy(9)-N(22)	88.8(7)
O(62)-Dy(3)-O(4)	132.4(8)	N(22)-Dy(9)-N(42)#3	136.0(6)
O(3)-Dy(4)-O(14)	143.1(6)	O(75)-Dy(10)-N(21)#1	74.3(7)
O(3)-Dy(4)-O(36)	83.8(6)	O(75)-Dy(10)-O(78)	139.1(8)
O(3)-Dy(4)-N(13)	74.2(7)	O(75)-Dy(10)-N(24)	69.6(7)

O(3)-Dy(4)-N(1A)	69.7(6)	O(75)-Dy(10)-O(64A)	143.9(8)
O(8)-Dy(4)-O(3)	71.6(7)	O(75)-Dy(10)-O(73A)	84.4(8)
O(8)-Dy(4)-O(14)	140.2(7)	O(78)-Dy(10)-N(21)#1	74.1(7)
O(8)-Dy(4)-O(36)	147.0(7)	O(78)-Dy(10)-N(24)	148.4(7)
O(8)-Dy(4)-N(13)	80.4(8)	O(78)-Dy(10)-O(64A)	75.1(9)
O(8)-Dy(4)-N(1A)	110.7(7)	O(85)-Dy(10)-N(21)#1	145.9(8)
O(14)-Dy(4)-N(13)	120.6(7)	O(85)-Dy(10)-O(75)	116.3(10)
O(14)-Dy(4)-N(1A)	78.9(6)	O(85)-Dy(10)-O(78)	79.2(9)
O(20)-Dy(4)-O(3)	119.4(7)	O(85)-Dy(10)-N(24)	73.9(8)
O(20)-Dy(4)-O(8)	75.8(7)	O(85)-Dy(10)-O(87)	66.5(11)
O(20)-Dy(4)-O(14)	69.0(6)	O(85)-Dy(10)-O(64A)	74.1(10)
O(20)-Dy(4)-O(36)	136.8(6)	O(85)-Dy(10)-O(73A)	137.1(9)
O(20)-Dy(4)-N(13)	145.9(7)	N(24)-Dy(10)-N(21)#1	136.8(6)
O(20)-Dy(4)-N(1A)	76.4(6)	N(24)-Dy(10)-O(64A)	81.9(8)
O(32)-Dy(4)-O(3)	140.0(7)	O(87)-Dy(10)-N(21)#1	87.0(9)
O(32)-Dy(4)-O(8)	77.8(8)	O(87)-Dy(10)-O(75)	75.8(9)
O(32)-Dy(4)-O(14)	75.9(7)	O(87)-Dy(10)-O(78)	77.4(9)
O(32)-Dy(4)-O(20)	75.5(8)	O(87)-Dy(10)-N(24)	105.8(9)
O(32)-Dy(4)-O(36)	111.1(8)	O(87)-Dy(10)-O(64A)	135.2(10)
O(32)-Dy(4)-N(13)	75.9(8)	O(87)-Dy(10)-O(73A)	155.3(9)
O(32)-Dy(4)-N(1A)	147.4(7)	O(64A)-Dy(10)-N(21)#1	117.7(8)
O(36)-Dy(4)-O(14)	71.5(6)	O(73A)-Dy(10)-N(21)#1	73.4(7)
O(36)-Dy(4)-N(13)	71.8(7)	O(73A)-Dy(10)-O(78)	110.4(8)
O(36)-Dy(4)-N(1A)	79.4(6)	O(73A)-Dy(10)-N(24)	80.1(7)
N(1A)-Dy(4)-N(13)	135.7(7)	O(73A)-Dy(10)-O(64A)	68.8(8)
O(7)-Dy(5)-O(17)	99.8(6)	O(31)-Dy(11)-O(49)	109.2(8)
O(7)-Dy(5)-O(27)	72.1(6)	O(31)-Dy(11)-O(51)	140.3(8)
O(7)-Dy(5)-O(34)	74.0(6)	O(31)-Dy(11)-O(52)	73.4(8)
O(7)-Dy(5)-O(47)	75.4(6)	O(31)-Dy(11)-N(36)	146.5(8)
O(7)-Dy(5)-O(48)	148.4(7)	O(31)-Dy(11)-O(81)	78.1(9)
O(17)-Dy(5)-O(27)	72.8(7)	O(31)-Dy(11)-O(84)	75.1(8)
O(17)-Dy(5)-O(34)	146.2(7)	O(31)-Dy(11)-N(47)	73.1(7)
O(17)-Dy(5)-O(47)	76.0(8)	O(49)-Dy(11)-O(51)	83.5(8)
O(17)-Dy(5)-O(48)	70.4(8)	O(49)-Dy(11)-O(52)	69.0(7)
O(27)-Dy(5)-O(48)	128.5(7)	O(49)-Dy(11)-N(36)	81.2(7)
O(30)-Dy(5)-O(7)	135.0(6)	O(49)-Dy(11)-O(81)	143.9(9)
O(30)-Dy(5)-O(17)	94.3(7)	O(49)-Dy(11)-N(47)	70.9(8)
O(30)-Dy(5)-O(27)	71.8(6)	O(51)-Dy(11)-O(52)	143.8(7)
O(30)-Dy(5)-O(34)	70.8(6)	O(51)-Dy(11)-N(47)	76.4(8)
O(30)-Dy(5)-O(47)	149.5(6)	O(52)-Dy(11)-N(47)	113.7(7)
O(30)-Dy(5)-O(48)	76.4(7)	N(36)-Dy(11)-O(51)	70.9(8)
O(30)-Dy(5)-O(65)	100.2(7)	N(36)-Dy(11)-O(52)	81.7(7)
O(34)-Dy(5)-O(27)	73.7(7)	N(36)-Dy(11)-N(47)	138.9(7)
O(34)-Dy(5)-O(47)	131.2(7)	O(81)-Dy(11)-O(51)	71.3(9)
O(34)-Dy(5)-O(48)	130.6(8)	O(81)-Dy(11)-O(52)	143.4(9)
O(47)-Dy(5)-O(27)	129.6(8)	O(81)-Dy(11)-N(36)	112.7(8)
O(47)-Dy(5)-O(48)	73.1(7)	O(81)-Dy(11)-N(47)	78.3(9)
O(65)-Dy(5)-O(7)	96.0(7)	O(84)-Dy(11)-O(49)	137.8(8)
O(65)-Dy(5)-O(17)	139.6(7)	O(84)-Dy(11)-O(51)	120.8(9)

O(65)-Dy(5)-O(27)	147.6(7)	O(84)-Dy(11)-O(52)	72.7(7)
O(65)-Dy(5)-O(34)	74.1(7)	O(84)-Dy(11)-N(36)	76.4(7)
O(65)-Dy(5)-O(47)	72.4(8)	O(84)-Dy(11)-O(81)	78.2(9)
O(65)-Dy(5)-O(48)	76.7(8)	O(84)-Dy(11)-N(47)	143.5(7)
O(1)-Dy(6)-O(19)	143.3(7)	O(35)-Dy(12)-N(40)	82.8(8)
O(1)-Dy(6)-O(46)	78.9(7)	O(56)-Dy(12)-O(35)	68.2(9)
O(1)-Dy(6)-N(6)	79.1(6)	O(56)-Dy(12)-O(77)	71.4(10)
O(1)-Dy(6)-N(11)	113.9(7)	O(56)-Dy(12)-N(40)	83.1(8)
O(19)-Dy(6)-O(46)	71.8(7)	O(56)-Dy(12)-N(45)#4	110.9(9)
O(19)-Dy(6)-N(6)	113.5(6)	O(57)-Dy(12)-O(35)	82.4(9)
O(19)-Dy(6)-N(11)	81.1(6)	O(57)-Dy(12)-O(56)	144.2(9)
O(22)-Dy(6)-O(1)	143.9(6)	O(57)-Dy(12)-O(67)	136.3(10)
O(22)-Dy(6)-O(19)	70.5(6)	O(57)-Dy(12)-O(77)	125.1(11)
O(22)-Dy(6)-O(46)	136.5(6)	O(57)-Dy(12)-O(86)	72.9(10)
O(22)-Dy(6)-N(6)	72.2(6)	O(57)-Dy(12)-N(40)	73.2(9)
O(22)-Dy(6)-N(11)	76.3(6)	O(57)-Dy(12)-N(45)#4	74.9(9)
O(25)-Dy(6)-O(1)	72.0(7)	O(67)-Dy(12)-O(35)	111.0(9)
O(25)-Dy(6)-O(19)	142.8(6)	O(67)-Dy(12)-O(56)	75.6(8)
O(25)-Dy(6)-O(22)	80.6(7)	O(67)-Dy(12)-O(77)	74.5(9)
O(25)-Dy(6)-O(46)	120.7(8)	O(67)-Dy(12)-O(86)	75.2(9)
O(25)-Dy(6)-N(6)	77.4(6)	O(67)-Dy(12)-N(40)	147.1(8)
O(25)-Dy(6)-N(11)	69.6(6)	O(67)-Dy(12)-N(45)#4	72.0(8)
O(41)-Dy(6)-O(1)	78.2(7)	O(77)-Dy(12)-O(35)	135.8(9)
O(41)-Dy(6)-O(19)	73.3(6)	O(77)-Dy(12)-N(40)	75.2(8)
O(41)-Dy(6)-O(22)	112.8(8)	O(86)-Dy(12)-O(35)	146.7(9)
O(41)-Dy(6)-O(25)	141.5(6)	O(86)-Dy(12)-O(56)	141.8(10)
O(41)-Dy(6)-O(46)	75.2(7)	O(86)-Dy(12)-O(77)	77.4(10)
O(41)-Dy(6)-N(6)	73.5(6)	O(86)-Dy(12)-N(40)	109.9(8)
O(41)-Dy(6)-N(11)	147.1(6)	O(86)-Dy(12)-N(45)#4	82.6(9)
O(46)-Dy(6)-N(6)	144.7(6)	N(45)#4-Dy(12)-O(35)	69.5(7)
O(46)-Dy(6)-N(11)	77.4(6)	N(45)#4-Dy(12)-O(77)	144.4(8)
N(11)-Dy(6)-N(6)	137.2(6)	N(45)#4-Dy(12)-N(40)	140.0(7)

Symmetry transformations used to generate equivalent atoms:

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

Table S3. Selected bond distances (Å) and angles (°) for compound **1(300K)**.

Bond distances			
Gd(1)-O(7)	2.420(10)	Gd(3A)-O(5A)	2.38(3)
Gd(1)-O(17)	2.344(8)	Gd(3A)-N(11)	2.531(15)
Gd(1)-O(18)	2.429(8)	Gd(3A)-O(2B)	2.39(3)
Gd(1)-O(3)	2.343(9)	Gd(3A)-O(4A)	2.34(3)
Gd(1)-O(8)	2.330(9)	Gd(3A)-O(3A)	2.40(3)
Gd(1)-O(9)	2.381(9)	Gd(3A)-N(12)#2	2.317(15)
Gd(1)-O(13)	2.332(9)	O(3)-N(9)	1.327(14)
Gd(1)-O(14)	2.399(9)	O(8)-N(4)	1.311(13)
Gd(2)-O(4)	2.349(9)	N(8)-O(15)	1.247(15)
Gd(2)-O(5)	2.395(10)	O(1)-Gd(3B)	2.306(18)
Gd(2)-O(6)	2.331(11)	N(10)-O(16)	1.279(16)
Gd(2)-O(10)	2.437(10)	N(11)-Gd(3B)	2.382(17)
Gd(2)-O(11)	2.335(9)	N(12)-Gd(3B)#3	2.559(10)
Gd(2)-O(12)	2.337(10)	Gd(3B)-O(6B)	2.39(4)
Gd(2)-N(1)#1	2.507(11)	Gd(3B)-O(5B)	2.38(4)
Angles			
O7-Gd1-O18	74.8(2)	O12-Gd2-N3	112.0(2)
O17-Gd1-O7	72.1(2)	N3-Gd2-N11	138.8(3)
O17-Gd1-O18	72.1(2)	O6A-Gd3-O1	85.6(4)
O17-Gd1-O9	149.1(2)	O6A-Gd3-O5A	69.5(5)
O17-Gd1-O13	133.6(2)	O6A-Gd3-N11	84.6(4)
O17-Gd1-O14	76.2(2)	O6A-Gd3-O2	148.3(4)
O3-Gd1-O7	147.4(2)	O6A-Gd3-O4A	136.7(7)
O3-Gd1-O17	100.3(2)	O6A-Gd3-O3A	107.9(5)
O3-Gd1-O18	72.7(2)	O6A-Gd3-N122	76.9(4)
O3-Gd1-O9	73.0(2)	O1-Gd3-O5A	144.5(5)
O3-Gd1-O13	94.6(2)	O1-Gd3-N11	70.8(3)
O3-Gd1-O14	77.3(2)	O1-Gd3-O2	68.0(3)
O8-Gd1-O7	71.6(2)	O1-Gd3-O4A	121.3(6)
O8-Gd1-O17	93.7(2)	O5A-Gd3-N11	81.8(5)
O8-Gd1-O18	146.2(2)	O5A-Gd3-O2	141.8(5)
O8-Gd1-O3	141.0(2)	O2-Gd3-N11	101.9(4)
O8-Gd1-O9	76.3(2)	O4A-Gd3-O5A	70.0(8)
O8-Gd1-O13	101.7(2)	O4A-Gd3-N11	75.1(4)
O8-Gd1-O14	71.0(2)	O4A-Gd3-O2	74.4(7)
O9-Gd1-O7	129.1(2)	O3A-Gd3-O1	140.4(4)
O9-Gd1-O18	130.4(2)	O3A-Gd3-O5A	73.4(6)
O9-Gd1-O14	72.9(2)	O3A-Gd3-N11	145.5(4)
O13-Gd1-O7	71.9(2)	O3A-Gd3-O2	84.3(5)
O13-Gd1-O18	70.98(19)	O3A-Gd3-O4A	74.1(5)
O13-Gd1-O9	77.3(2)	O3A-Gd3-N122	71.7(4)
O13-Gd1-O14	150.2(2)	N122-Gd3-O1	75.7(3)
O14-Gd1-O7	128.4(2)	N122-Gd3-O5A	120.0(5)
O14-Gd1-O18	130.9(2)	N122-Gd3-N11	142.7(3)
O4-Gd2-O5	82.7(2)	N122-Gd3-O2	79.6(4)
O4-Gd2-O10	142.4(2)	N122-Gd3-O4A	138.6(5)

O4-Gd2-N11	74.6(2)	O1-Gd2A-N122	67.2(3)
O4-Gd2-N3	72.3(2)	N11-Gd2A-O1	75.1(4)
O5-Gd2-O10	70.1(2)	N11-Gd2A-N122	129.8(5)
O5-Gd2-N11	72.4(2)	N11-Gd2A-O6B	69.3(9)
O5-Gd2-N3	79.7(2)	O2-Gd2A-O1	73.8(5)
O6-Gd2-O4	121.8(2)	O2-Gd2A-N11	123.8(6)
O6-Gd2-O5	138.2(2)	O2-Gd2A-N122	75.9(5)
O6-Gd2-O10	71.1(2)	O2-Gd2A-O6B	135.2(10)
O6-Gd2-O11	73.7(2)	O2-Gd2A-O5B	150.7(12)
O6-Gd2-O12	75.8(2)	O2-Gd2A-O3B	74.3(13)
O6-Gd2-N11	142.4(2)	O6B-Gd2A-O1	69.2(9)
O6-Gd2-N3	77.3(2)	O5B-Gd2A-O1	135.4(12)
O10-Gd2-N11	118.5(2)	O5B-Gd2A-N11	75.6(11)
O10-Gd2-N3	77.5(2)	O5B-Gd2A-O6B	69.4(14)
O11-Gd2-O4	139.3(2)	O5B-Gd2A-O3B	79.6(16)
O11-Gd2-O5	111.1(2)	O4B-Gd2A-O1	133.8(16)
O11-Gd2-O10	76.5(2)	O4B-Gd2A-N11	81.0(14)
O11-Gd2-N11	73.9(2)	O4B-Gd2A-O2	88(2)
O11-Gd2-N3	146.0(2)	O4B-Gd2A-O6B	136(2)
O12-Gd2-O4	71.6(2)	O4B-Gd2A-O5B	72(2)
O12-Gd2-O5	145.8(2)	O4B-Gd2A-O3B	75.3(16)
O12-Gd2-O10	142.5(2)	O3B-Gd2A-O1	135.1(11)
O12-Gd2-O11	77.8(2)	O3B-Gd2A-N11	149.8(11)
O12-Gd2-N11	79.2(3)	O3B-Gd2A-O6B	117.1(15)

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Selected bond distances (Å) and angles (°) for compound **2(300K)**.

Bond distances			
Dy(1)-O(7)	2.419(8)	Dy(3A)-O(5A)	2.48(2)
Dy(1)-O(17)	2.345(7)	Dy(3A)-N(11)	2.549(12)
Dy(1)-O(18)	2.425(7)	Dy(3A)-O(2B)	2.33(3)
Dy(1)-O(3)	2.341(8)	Dy(3A)-O(4A)	2.41(2)
Dy(1)-O(8)	2.339(7)	Dy(3A)-O(3A)	2.372(19)
Dy(1)-O(9)	2.395(7)	Dy(3A)-N(12)#2	2.378(13)
Dy(1)-O(13)	2.338(7)	O(3)-N(9)	1.312(11)
Dy(1)-O(14)	2.398(7)	O(8)-N(4)	1.320(11)
Dy(2)-O(4)	2.362(7)	N(8)-O(15)	1.260(12)
Dy(2)-O(5)	2.381(8)	O(1)-Dy(3B)	2.386(16)
Dy(2)-O(6)	2.335(8)	N(10)-O(16)	1.276(13)
Dy(2)-O(10)	2.434(8)	N(11)-Dy(3B)	2.352(15)
Dy(2)-O(11)	2.331(7)	N(12)-Dy(3B)#3	2.760(16)
Dy(2)-O(12)	2.348(8)	Dy(3B)-O(6B)	2.37(3)
Dy(2)-N(1)#1	2.505(9)	Dy(3B)-O(5B)	2.24(4)
Angles			
O7-Dy1-O18	74.97(17)	O12-Dy2-N3	112.1(2)
O17-Dy1-O7	72.25(17)	N3-Dy2-N11	138.8(2)
O17-Dy1-O18	72.22(17)	O6A-Dy3A-O1	84.3(4)
O17-Dy1-O9	149.13(17)	O6A-Dy3A-O5A	70.2(5)
O17-Dy1-O13	133.86(18)	O6A-Dy3A-N11	84.1(4)
O17-Dy1-O14	75.78(18)	O6A-Dy3A-O2	147.9(4)
O3-Dy1-O7	147.33(18)	O6A-Dy3A-O4A	136.3(5)
O3-Dy1-O17	100.38(17)	O6A-Dy3A-N122	76.5(4)
O3-Dy1-O18	72.51(18)	O1-Dy3A-O5A	143.3(4)
O3-Dy1-O9	73.01(19)	O1-Dy3A-N11	70.5(2)
O3-Dy1-O13	94.33(17)	O1-Dy3A-O2	68.9(3)
O3-Dy1-O14	77.43(19)	O5A-Dy3A-N11	80.8(4)
O8-Dy1-O7	71.66(18)	O2-Dy3A-O5A	141.6(4)
O8-Dy1-O17	93.61(17)	O2-Dy3A-N11	102.2(3)
O8-Dy1-O18	146.39(19)	O4A-Dy3A-O1	122.6(4)
O8-Dy1-O3	141.00(19)	O4A-Dy3A-O5A	68.6(5)
O8-Dy1-O9	76.38(19)	O4A-Dy3A-N11	75.5(3)
O8-Dy1-O13	101.79(17)	O4A-Dy3A-O2	75.1(4)
O8-Dy1-O14	71.0(2)	O4A-Dy3A-N122	139.0(4)
O9-Dy1-O7	128.96(18)	O3A-Dy3A-O6A	109.5(4)
O9-Dy1-O18	130.28(17)	O3A-Dy3A-O1	140.5(3)
O13-Dy1-O7	71.99(18)	O3A-Dy3A-O5A	74.7(5)
O13-Dy1-O18	71.09(17)	O3A-Dy3A-N11	145.3(3)
O13-Dy1-O9	77.01(17)	O3A-Dy3A-O2	83.2(4)
O13-Dy1-O14	150.36(18)	O3A-Dy3A-O4A	72.9(4)
O14-Dy1-O7	128.30(18)	O3A-Dy3A-N122	72.3(3)
O14-Dy1-O18	130.52(19)	N122-Dy3A-O1	75.5(3)
O14-Dy1-O9	73.35(18)	N122-Dy3A-O5A	120.9(5)
O4-Dy2-O5	82.61(18)	N122-Dy3A-N11	142.3(3)
O4-Dy2-O10	142.54(18)	N122-Dy3A-O2	79.8(3)

O4-Dy2-N11	74.5(2)	O1-Dy3B-N122	67.5(3)
O4-Dy2-N3	72.42(19)	N11-Dy3B-O1	75.2(4)
O5-Dy2-O10	70.14(19)	N11-Dy3B-N122	129.4(4)
O5-Dy2-N11	72.59(19)	N11-Dy3B-O6B	68.9(9)
O5-Dy2-N3	79.43(19)	O2-Dy3B-O1	76.2(4)
O6-Dy2-O4	121.7(2)	O2-Dy3B-N11	126.2(6)
O6-Dy2-O5	138.23(19)	O2-Dy3B-N122	76.6(4)
O6-Dy2-O10	71.2(2)	O2-Dy3B-O6B	136.2(9)
O6-Dy2-O12	75.9(2)	O2-Dy3B-O5B	148.6(11)
O6-Dy2-N11	142.3(2)	O2-Dy3B-O4B	83.4(12)
O6-Dy2-N3	77.4(2)	O2-Dy3B-O3B	69.5(10)
O10-Dy2-N11	118.4(2)	O6B-Dy3B-O1	68.7(9)
O10-Dy2-N3	77.57(19)	O5B-Dy3B-O1	134.3(11)
O11-Dy2-O4	138.98(18)	O5B-Dy3B-N11	77.4(10)
O11-Dy2-O5	111.24(19)	O5B-Dy3B-O6B	67.7(13)
O11-Dy2-O6	73.9(2)	O5B-Dy3B-O4B	79.7(15)
O11-Dy2-O10	76.61(19)	O5B-Dy3B-O3B	79.8(14)
O11-Dy2-O12	77.8(2)	O4B-Dy3B-O1	130.4(11)
O11-Dy2-N11	73.6(2)	O4B-Dy3B-N11	81.9(11)
O11-Dy2-N3	146.3(2)	O4B-Dy3B-O6B	139.8(14)
O12-Dy2-O4	71.3(2)	O4B-Dy3B-O3B	69.7(14)
O12-Dy2-O5	145.6(2)	O3B-Dy3B-O1	137.6(9)
O12-Dy2-O10	142.7(2)	O3B-Dy3B-N11	146.2(9)
O12-Dy2-N11	78.9(2)	O3B-Dy3B-O6B	123.6(14)

Symmetry transformations used to generate equivalent atoms:

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

Table S5. SHAPE analyses for **1**and**2**.

1	Gd1	Gd2	Gd3	Gd4	Gd5	Gd6	Gd7	Gd8	Gd9	Gd10	Gd11	Gd12
SAPR-8	2.486	2.321	2.211	2.787	**0.618**	**0.367**	**0.446**	**0.519**	1.410	**0.905**	**0.480**	**0.691**
TDD-8	**0.230**	**0.106**	**0.163**	**0.133**	2.338	2.133	2.150	2.008	**1.133**	2.108	2.256	1.788
BTPR-8	2.657	2.464	2.185	2.657	2.114	2.285	2.046	1.954	1.551	1.699	2.243	2.222
2	Dy1	Dy2	Dy3	Dy4	Dy5	Dy6	Dy7	Dy8	Dy9	Dy10	Dy11	Dy12
SAPR-8	2.364	2.210	2.534	2.671	**0.824**	**0.307**	**0.392**	**0.447**	1.469	**0.653**	**0.597**	**0.316**
TDD-8	**0.072**	**0.160**	**0.101**	**0.202**	2.192	2.288	1.938	2.377	**1.053**	2.006	2.516	2.118
BTPR-8	2.412	2.115	2.489	2.879	1.847	2.295	1.891	2.150	1.629	2.197	2.111	1.968

SAPR-8: Square antiprism; TDD-8: Triangular dodecahedron; BTPR-8: Biaugmented trigonal prism

Table S6. Key bond lengths (Å) and angles (deg) for **1** and **2** at 113K and 300K.

Complex	**1(113K)**	**2(113K)**	**1(300K)**	**2(300K)**
Ln–O_{rad}	2.37(2)–2.43(2)	2.31(2)–2.41(2)	2.306(18),2.343(9)	2.386(16), 2.341(8)
Ln–O_{hfac}	2.28(2)−2.480(16)	2.21(3)–2.403(19)	2.331(11)–2.437(10)	2.24(4)–2.48(2)
Ln–N	2.404(11)–2.543(12)	2.382(13)–2.512(16)	2.317(15),2.559(10)	2.378(13), 2.549(12)
O_{rad}–Ln–O_{rad}	140.1(3) –148.6 (5)	139.3(2) –148.3(1)	141.8(5)	141.1(6)
Ln–O–N	129.8(5) –136.7(8)	129.3(5) –136.4(9)	138.4(5), 138.2(7)	137.2(9), 138.3(8)

Table S7. Cell parameters of complex **1** at various temperatures.

Temperature/K	120	130	140	150
a/Å	27.18(8)	29.71(7)	29.46(5)	25.77(7)
b/Å	22.88(5)	22.55(5)	22.78(5)	21.73(6)
c/Å	39.54(7)	39.80(9)	39.47(6)	40.25(13)
α/°	90	90	90	89.8(2)
β/°	95.06(19)	95.38(19)	95.24(13)	94.0(2)
γ/°	90	90	90	92.5(5)
Volume/Å^3	24496(90)	26536(100)	26382(80)	22472(20)
Z	2	2	2	–
Temperature/K	170	200	250	300
a/Å	25.78(6)	25.95(6)	26.08(3)	26.0907(8)
b/Å	22.71(5)	22.41(5)	22.93(3)	23.0966(6)
c/Å	23.67(6)	23.67(6)	23.69(4)	23.9398(10)
α/°	90	90	90	90
β/°	106.7(2)	106.8(3)	105.99(17)	107.288(4)
γ/°	90	90	90	90
Volume/Å^3	22472(20)	13198(60)	13602(40)	13774.5(8)
Z	4	4	4	4