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Syntheses, structures and magnetic properties of a series of mono- and di- nuclear dysprosium(III)-crown-ether complexes: effects of weak ligand-field and flexible cyclic coordination modes

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1 Crystallographic data

Table S1, Bond lengths (Å) for complex **1**

Dy(1)-O(7)	2.387(11)	Dy(1)-N(3)	2.853(13)	N(3)-O(9)	1.273(17)
Dy(1)-O(5)	2.401(10)	O(1)-C(3)	1.47(2)	N(2)-O(8)	1.222(18)
Dy(1)-O(3)	2.447(9)	O(1)-C(2)	1.474(19)	N(2)-O(7)	1.262(18)
Dy(1)-O(9)	2.456(11)	O(2)-C(5)	1.425(18)	N(2)-O(12)	1.270(17)
Dy(1)-O(10)	2.460(10)	O(2)-C(4)	1.440(18)	N(1)-O(13)	1.207(16)
Dy(1)-O(4)	2.460(10)	O(4)-C(8)	1.442(17)	N(1)-O(5)	1.258(17)
Dy(1)-O(6)	2.479(11)	O(4)-C(1)	1.45(2)	N(1)-O(6)	1.267(17)
Dy(1)-O(8)	2.480(11)	O(3)-C(6)	1.411(17)	C(4)-C(3)	1.50(2)
Dy(1)-O(1)	2.517(11)	O(3)-C(7)	1.431(18)	C(6)-C(5)	1.50(2)
Dy(1)-O(2)	2.547(9)	N(3)-O(11)	1.219(17)	C(1)-C(2)	1.45(3)
Dy(1)-N(2)	2.851(13)	N(3)-O(10)	1.251(18)	C(8)-C(7)	1.48(2)

Table S2,Angles (deg) for complex **1**

O(7)-Dy(1)-O(5)	77.2(4)	O(7)-Dy(1)-N(3)	133.4(4)
O(7)-Dy(1)-O(3)	129.5(4)	O(5)-Dy(1)-N(3)	102.6(4)
O(5)-Dy(1)-O(3)	72.4(3)	O(3)-Dy(1)-N(3)	92.5(4)
O(7)-Dy(1)-O(9)	143.4(4)	O(9)-Dy(1)-N(3)	26.4(4)
O(5)-Dy(1)-O(9)	82.5(4)	O(10)-Dy(1)-N(3)	25.9(4)
O(3)-Dy(1)-O(9)	70.1(4)	O(4)-Dy(1)-N(3)	154.7(3)
O(7)-Dy(1)-O(10)	116.4(4)	O(6)-Dy(1)-N(3)	71.7(4)
O(5)-Dy(1)-O(10)	121.8(4)	O(8)-Dy(1)-N(3)	88.7(4)
O(3)-Dy(1)-O(10)	113.8(3)	O(1)-Dy(1)-N(3)	114.9(4)
O(9)-Dy(1)-O(10)	52.3(4)	O(2)-Dy(1)-N(3)	72.8(3)
O(7)-Dy(1)-O(4)	71.9(4)	N(2)-Dy(1)-N(3)	111.0(4)
O(5)-Dy(1)-O(4)	82.2(4)	C(3)-O(1)-C(2)	115.6(12)
O(3)-Dy(1)-O(4)	64.9(3)	C(3)-O(1)-Dy(1)	107.7(9)
O(9)-Dy(1)-O(4)	135.0(4)	C(2)-O(1)-Dy(1)	117.1(9)
O(10)-Dy(1)-O(4)	155.2(4)	C(5)-O(2)-C(4)	113.9(12)
O(7)-Dy(1)-O(6)	72.6(4)	C(5)-O(2)-Dy(1)	121.0(9)
O(5)-Dy(1)-O(6)	51.9(4)	C(4)-O(2)-Dy(1)	118.3(8)
O(3)-Dy(1)-O(6)	114.4(4)	C(8)-O(4)-C(1)	112.7(12)
O(9)-Dy(1)-O(6)	70.9(4)	C(8)-O(4)-Dy(1)	120.3(9)
O(10)-Dy(1)-O(6)	77.3(4)	C(1)-O(4)-Dy(1)	114.6(9)
O(4)-Dy(1)-O(6)	126.7(4)	C(6)-O(3)-C(7)	118.2(11)
O(7)-Dy(1)-O(8)	51.3(4)	C(6)-O(3)-Dy(1)	116.9(8)
O(5)-Dy(1)-O(8)	111.9(4)	C(7)-O(3)-Dy(1)	115.9(8)
O(3)-Dy(1)-O(8)	175.2(4)	O(11)-N(3)-O(10)	121.7(15)
O(9)-Dy(1)-O(8)	112.1(4)	O(11)-N(3)-O(9)	120.0(15)
O(10)-Dy(1)-O(8)	66.2(4)	O(10)-N(3)-O(9)	118.3(12)
O(4)-Dy(1)-O(8)	112.9(4)	O(11)-N(3)-Dy(1)	177.9(11)
O(6)-Dy(1)-O(8)	70.4(4)	O(10)-N(3)-Dy(1)	59.2(7)
O(7)-Dy(1)-O(1)	74.7(4)	O(9)-N(3)-Dy(1)	59.1(7)
O(5)-Dy(1)-O(1)	142.4(4)	O(8)-N(2)-O(7)	116.1(12)
O(3)-Dy(1)-O(1)	107.9(3)	O(8)-N(2)-O(12)	121.0(16)

O(9)-Dy(1)-O(1)	134.2(4)	O(7)-N(2)-O(12)	122.8(15)
O(10)-Dy(1)-O(1)	93.2(4)	O(8)-N(2)-Dy(1)	60.1(7)
O(4)-Dy(1)-O(1)	65.5(4)	O(7)-N(2)-Dy(1)	56.0(7)
O(6)-Dy(1)-O(1)	136.9(4)	O(12)-N(2)-Dy(1)	178.6(12)
O(8)-Dy(1)-O(1)	67.4(4)	O(13)-N(1)-O(5)	121.5(15)
O(7)-Dy(1)-O(2)	138.5(4)	O(13)-N(1)-O(6)	122.5(14)
O(5)-Dy(1)-O(2)	135.5(3)	O(5)-N(1)-O(6)	115.8(11)
O(3)-Dy(1)-O(2)	63.8(3)	O(13)-N(1)-Dy(1)	177.0(13)
O(9)-Dy(1)-O(2)	75.9(4)	O(5)-N(1)-Dy(1)	56.1(6)
O(10)-Dy(1)-O(2)	72.3(3)	O(6)-N(1)-Dy(1)	59.7(7)
O(4)-Dy(1)-O(2)	86.3(3)	N(2)-O(8)-Dy(1)	94.6(9)
O(6)-Dy(1)-O(2)	144.3(4)	N(1)-O(5)-Dy(1)	98.1(8)
O(8)-Dy(1)-O(2)	112.2(4)	N(3)-O(10)-Dy(1)	94.9(8)
O(1)-Dy(1)-O(2)	64.1(3)	N(3)-O(9)-Dy(1)	94.5(9)
O(7)-Dy(1)-N(2)	26.0(4)	N(1)-O(6)-Dy(1)	94.1(8)
O(5)-Dy(1)-N(2)	94.6(4)	N(2)-O(7)-Dy(1)	98.0(9)
O(3)-Dy(1)-N(2)	155.3(4)	O(2)-C(4)-C(3)	110.2(12)
O(9)-Dy(1)-N(2)	130.2(4)	O(3)-C(6)-C(5)	111.5(12)
O(10)-Dy(1)-N(2)	90.9(4)	O(1)-C(3)-C(4)	109.8(13)
O(4)-Dy(1)-N(2)	93.1(4)	O(2)-C(5)-C(6)	106.8(13)
O(6)-Dy(1)-N(2)	68.8(4)	O(4)-C(1)-C(2)	109.8(14)
O(8)-Dy(1)-N(2)	25.3(4)	O(4)-C(8)-C(7)	105.4(12)
O(1)-Dy(1)-N(2)	69.5(4)	O(3)-C(7)-C(8)	109.7(13)
O(2)-Dy(1)-N(2)	129.0(4)	C(1)-C(2)-O(1)	106.7(13)

Table S3, Bond lengths (Å) for complex **2**

Dy(1)-N(1)	2.369(18)	O(3)-Cl(1)	1.461(10)	O(15)-C(5)	1.469(16)
Dy(1)-O(14)#1	2.383(10)	O(5)-Cl(2)	1.503(16)	O(16)-C(7)	1.439(19)
Dy(1)-O(14)	2.383(10)	O(6)-Cl(2)	1.364(12)	O(16)-C(6)	1.53(2)
Dy(1)-O(13)#1	2.399(11)	O(7)-Cl(2)	1.352(18)	Cl(1)-O(3)#2	1.461(10)
Dy(1)-O(13)	2.399(11)	O(8)-Cl(2)	1.427(18)	Cl(1)-O(1)#2	1.467(12)
Dy(1)-O(16)#1	2.406(8)	O(13)-C(1)	1.47(3)	C(1)-C(2)	1.25(3)
Dy(1)-O(16)	2.406(8)	O(13)-C(8)	1.47(2)	C(3)-C(4)	1.51(2)
Dy(1)-O(15)	2.467(10)	O(14)-C(2)	1.44(2)	C(5)-C(6)	1.44(3)
Dy(1)-O(15)#1	2.467(10)	O(14)-C(3)	1.476(18)	C(7)-C(8)	1.45(3)
N(1)-C(17)	1.17(3)	O(15)-C(4)	1.36(2)	C(17)-C(18)	1.32(6)
O(1)-Cl(1)	1.467(12)				

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

Table S4, Angles (deg) for complex **2**

N(1)-Dy(1)-O(14)#1	115.2(3)	O(15)-Dy(1)-O(15)#1	140.1(5)
N(1)-Dy(1)-O(14)	115.2(3)	C(17)-N(1)-Dy(1)	180.0(12)
O(14)#1-Dy(1)-O(14)	129.6(5)	C(1)-O(13)-C(8)	121.1(17)
N(1)-Dy(1)-O(13)#1	141.5(3)	C(1)-O(13)-Dy(1)	113.8(12)
O(14)#1-Dy(1)-O(13)#1	67.2(3)	C(8)-O(13)-Dy(1)	119.9(11)
O(14)-Dy(1)-O(13)#1	73.8(4)	C(2)-O(14)-C(3)	115.2(14)
N(1)-Dy(1)-O(13)	141.5(3)	C(2)-O(14)-Dy(1)	117.6(11)
O(14)#1-Dy(1)-O(13)	73.8(4)	C(3)-O(14)-Dy(1)	111.0(8)
O(14)-Dy(1)-O(13)	67.2(3)	C(4)-O(15)-C(5)	113.9(12)
O(13)#1-Dy(1)-O(13)	77.0(7)	C(4)-O(15)-Dy(1)	122.5(9)
N(1)-Dy(1)-O(16)#1	79.5(3)	C(5)-O(15)-Dy(1)	120.4(9)
O(14)#1-Dy(1)-O(16)#1	116.6(3)	C(7)-O(16)-C(6)	116.5(11)
O(14)-Dy(1)-O(16)#1	73.0(3)	C(7)-O(16)-Dy(1)	115.2(8)
O(13)#1-Dy(1)-O(16)#1	67.2(4)	C(6)-O(16)-Dy(1)	114.2(9)
O(13)-Dy(1)-O(16)#1	132.3(4)	O(3)#2-Cl(1)-O(3)	110.3(10)
N(1)-Dy(1)-O(16)	79.5(3)	O(3)#2-Cl(1)-O(1)#2	110.2(7)
O(14)#1-Dy(1)-O(16)	73.0(3)	O(3)-Cl(1)-O(1)#2	109.8(8)
O(14)-Dy(1)-O(16)	116.6(3)	O(3)#2-Cl(1)-O(1)	109.8(8)
O(13)#1-Dy(1)-O(16)	132.3(4)	O(3)-Cl(1)-O(1)	110.2(7)
O(13)-Dy(1)-O(16)	67.2(4)	O(1)#2-Cl(1)-O(1)	106.4(10)
O(16)#1-Dy(1)-O(16)	159.0(5)	O(7)-Cl(2)-O(6)	116.5(11)
N(1)-Dy(1)-O(15)	70.1(3)	O(7)-Cl(2)-O(8)	116.1(11)
O(14)#1-Dy(1)-O(15)	136.7(3)	O(6)-Cl(2)-O(8)	111.5(10)
O(14)-Dy(1)-O(15)	64.0(4)	O(7)-Cl(2)-O(5)	101.2(13)
O(13)#1-Dy(1)-O(15)	136.8(4)	O(6)-Cl(2)-O(5)	101.4(11)
O(13)-Dy(1)-O(15)	78.7(4)	O(8)-Cl(2)-O(5)	108.0(13)
O(16)#1-Dy(1)-O(15)	106.6(3)	C(2)-C(1)-O(13)	118(2)
O(16)-Dy(1)-O(15)	65.8(3)	C(1)-C(2)-O(14)	117(2)
N(1)-Dy(1)-O(15)#1	70.1(3)	O(14)-C(3)-C(4)	109.1(11)
O(14)#1-Dy(1)-O(15)#1	64.0(4)	O(15)-C(4)-C(3)	107.9(12)
O(14)-Dy(1)-O(15)#1	136.7(3)	C(6)-C(5)-O(15)	107.2(13)
O(13)#1-Dy(1)-O(15)#1	78.7(4)	C(5)-C(6)-O(16)	108.3(13)
O(13)-Dy(1)-O(15)#1	136.8(4)	O(16)-C(7)-C(8)	112.1(13)
O(16)#1-Dy(1)-O(15)#1	65.8(3)	C(7)-C(8)-O(13)	109.8(14)
O(16)-Dy(1)-O(15)#1	106.6(3)	N(1)-C(17)-C(18)	179.999(3)

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

Table S5, Bond lengths (Å) for complex **3**

Cl(1)-O(10)	1.426(3)	Dy(1)-O(7)	2.371(3)	O(2)-C(2)	1.450(5)
Cl(1)-O(11)	1.430(3)	Dy(1)-O(6)	2.383(3)	O(3)-C(5)	1.449(5)
Cl(1)-O(9)	1.443(3)	Dy(1)-O(2)	2.423(3)	O(3)-C(4)	1.451(5)
Cl(1)-O(8)	1.469(3)	Dy(1)-O(4)	2.425(3)	O(1)-C(1)	1.444(5)
Cl(3)-O(12)	1.369(4)	Dy(1)-O(1)	2.481(3)	O(1)-C(8)	1.451(4)
Cl(3)-O(15)	1.402(4)	Dy(1)-O(3)	2.496(3)	O(5)-Dy(1)#1	2.209(3)
Cl(3)-O(13)	1.419(3)	Dy(1)-Dy(1)#1	3.6353(4)	C(7)-C(8)	1.506(6)
Cl(3)-O(14)	1.501(5)	O(4)-C(7)	1.446(4)	C(5)-C(6)	1.515(5)
Dy(1)-O(5)#1	2.209(3)	O(4)-C(6)	1.452(4)	C(4)-C(3)	1.505(6)
Dy(1)-O(5)	2.249(3)	O(2)-C(3)	1.443(5)	C(2)-C(1)	1.510(6)

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

Table S6, Angles (deg) for complex **3**

O(10)-Cl(1)-O(11)	111.3(2)	O(7)-Dy(1)-O(3)	134.03(10)
O(10)-Cl(1)-O(9)	110.2(2)	O(6)-Dy(1)-O(3)	74.84(10)
O(11)-Cl(1)-O(9)	110.4(2)	O(2)-Dy(1)-O(3)	66.08(9)
O(10)-Cl(1)-O(8)	108.6(2)	O(4)-Dy(1)-O(3)	66.34(9)
O(11)-Cl(1)-O(8)	108.12(19)	O(1)-Dy(1)-O(3)	104.30(9)
O(9)-Cl(1)-O(8)	108.14(17)	O(5)#1-Dy(1)-Dy(1)#1	35.72(7)
O(12)-Cl(3)-O(15)	117.9(3)	O(5)-Dy(1)-Dy(1)#1	34.99(7)
O(12)-Cl(3)-O(13)	113.2(3)	O(7)-Dy(1)-Dy(1)#1	104.08(8)
O(15)-Cl(3)-O(13)	114.9(2)	O(6)-Dy(1)-Dy(1)#1	102.03(7)
O(12)-Cl(3)-O(14)	101.9(4)	O(2)-Dy(1)-Dy(1)#1	179.25(6)
O(15)-Cl(3)-O(14)	104.5(3)	O(4)-Dy(1)-Dy(1)#1	81.35(6)
O(13)-Cl(3)-O(14)	101.3(3)	O(1)-Dy(1)-Dy(1)#1	113.09(6)
O(5)#1-Dy(1)-O(5)	70.71(12)	O(3)-Dy(1)-Dy(1)#1	114.18(6)
O(5)#1-Dy(1)-O(7)	82.34(11)	C(7)-O(4)-C(6)	114.4(3)
O(5)-Dy(1)-O(7)	121.60(11)	C(7)-O(4)-Dy(1)	113.6(2)
O(5)#1-Dy(1)-O(6)	122.20(10)	C(6)-O(4)-Dy(1)	121.6(2)
O(5)-Dy(1)-O(6)	79.25(10)	C(3)-O(2)-C(2)	114.0(3)
O(7)-Dy(1)-O(6)	73.05(11)	C(3)-O(2)-Dy(1)	114.1(2)
O(5)#1-Dy(1)-O(2)	143.72(10)	C(2)-O(2)-Dy(1)	121.7(2)
O(5)-Dy(1)-O(2)	145.56(10)	C(5)-O(3)-C(4)	113.3(3)
O(7)-Dy(1)-O(2)	76.01(11)	C(5)-O(3)-Dy(1)	111.5(2)
O(6)-Dy(1)-O(2)	78.71(9)	C(4)-O(3)-Dy(1)	118.3(2)
O(5)#1-Dy(1)-O(4)	84.56(9)	C(1)-O(1)-C(8)	112.0(3)
O(5)-Dy(1)-O(4)	81.38(9)	C(1)-O(1)-Dy(1)	112.4(2)
O(7)-Dy(1)-O(4)	147.20(10)	C(8)-O(1)-Dy(1)	118.6(2)
O(6)-Dy(1)-O(4)	138.32(10)	Dy(1)#1-O(5)-Dy(1)	109.29(12)
O(2)-Dy(1)-O(4)	98.17(9)	Dy(1)#1-O(5)-H(9)	126(5)
O(5)#1-Dy(1)-O(1)	82.34(10)	O(4)-C(7)-C(8)	109.6(3)

O(5)-Dy(1)-O(1)	139.90(9)	O(3)-C(5)-C(6)	109.7(3)
O(7)-Dy(1)-O(1)	81.86(10)	O(4)-C(6)-C(5)	106.2(3)
O(6)-Dy(1)-O(1)	140.85(9)	O(3)-C(4)-C(3)	106.1(3)
O(2)-Dy(1)-O(1)	66.17(9)	O(1)-C(8)-C(7)	106.4(3)
O(4)-Dy(1)-O(1)	66.64(9)	O(2)-C(2)-C(1)	105.9(3)
O(5)#1-Dy(1)-O(3)	143.32(10)	O(2)-C(3)-C(4)	108.6(3)
O(5)-Dy(1)-O(3)	82.79(9)	O(1)-C(1)-C(2)	109.8(3)

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

Table S7, Bond lengths (Å) for complex **4**

Dy(1)-O(42)	2.366(2)	O(47)-C(24)	1.459(4)	O(63)-C(46)	1.451(4)
Dy(1)-O(43)	2.397(2)	O(48)-C(22)	1.449(4)	C(37)-C(38)	1.502(4)
Dy(1)-O(41)	2.417(2)	O(48)-C(21)	1.452(4)	C(39)-C(40)	1.490(5)
Dy(1)-O(45)	2.427(3)	O(49)-C(26)	1.452(4)	C(41)-C(42)	1.500(5)
Dy(1)-O(44)	2.445(2)	O(49)-C(20)	1.462(4)	C(43)-C(44)	1.508(4)
Dy(1)-O(39)	2.492(2)	O(50)-C(34)	1.442(4)	C(45)-C(46)	1.509(4)
Dy(1)-O(37)	2.512(2)	O(50)-C(35)	1.442(4)	C(47)-C(48)	1.511(5)
Dy(1)-O(38)	2.533(2)	O(51)-C(33)	1.452(4)	C(49)-C(50)	1.507(5)
Dy(1)-O(40)	2.603(2)	O(51)-C(32)	1.453(4)	C(51)-C(52)	1.495(5)
Dy(1)-N(2)	2.736(3)	O(52)-C(31)	1.442(4)	C(53)-C(54)	1.504(4)
O(37)-C(6)	1.440(4)	O(52)-C(30)	1.451(4)	Cl(1)-O(1)	1.425(3)
O(37)-C(7)	1.452(4)	O(53)-C(28)	1.447(4)	Cl(1)-O(3)	1.436(2)
O(38)-C(8)	1.444(4)	O(53)-C(29)	1.450(4)	Cl(1)-O(2)	1.440(2)
O(38)-C(1)	1.453(4)	O(54)-C(36)	1.447(4)	Cl(1)-O(4)	1.448(3)
O(39)-C(2)	1.445(4)	O(54)-C(27)	1.452(4)	Cl(2)-O(8)	1.419(3)
O(39)-C(3)	1.459(4)	C(19)-C(20)	1.501(4)	Cl(2)-O(5)	1.420(3)
O(40)-C(4)	1.437(5)	C(21)-C(26)	1.507(4)	Cl(2)-O(6)	1.434(3)
O(40)-C(5)	1.451(5)	C(22)-C(23)	1.514(4)	Cl(2)-O(7)	1.468(3)
O(41)-C(11)	1.435(4)	C(24)-C(25)	1.505(5)	Cl(3)-O(11)	1.428(3)
O(41)-C(10)	1.444(4)	C(27)-C(28)	1.523(5)	Cl(3)-O(12)	1.435(2)
O(42)-C(9)	1.439(4)	C(29)-C(30)	1.499(5)	Cl(3)-O(9)	1.439(3)
O(42)-C(18)	1.444(4)	C(31)-C(32)	1.516(4)	Cl(3)-O(10)	1.450(3)
O(43)-C(16)	1.434(4)	C(33)-C(34)	1.508(5)	Cl(4)-O(15)	1.433(2)
O(43)-C(17)	1.437(4)	C(35)-C(36)	1.505(5)	Cl(4)-O(14)	1.437(3)
O(44)-C(15)	1.420(4)	Dy(3)-O(60)	2.398(2)	Cl(4)-O(13)	1.438(3)
O(44)-C(14)	1.423(4)	Dy(3)-O(61)	2.399(2)	Cl(4)-O(16)	1.444(2)
O(45)-C(13)	1.429(4)	Dy(3)-O(63)	2.412(2)	Cl(5)-O(17)	1.405(3)
O(45)-C(12)	1.431(4)	Dy(3)-O(62)	2.413(2)	Cl(5)-O(19)	1.429(3)
C(14)-C(13)	1.530(5)	Dy(3)-O(59)	2.444(2)	Cl(5)-O(20)	1.433(3)
N(2)-C(57)	1.132(5)	Dy(3)-O(58)	2.448(2)	Cl(5)-O(18)	1.461(3)
C(1)-C(2)	1.494(6)	Dy(3)-O(55)	2.461(2)	Cl(6)-O(21)	1.430(3)
C(3)-C(4)	1.493(6)	Dy(3)-O(57)	2.478(2)	Cl(6)-O(24)	1.434(2)
C(5)-C(6)	1.494(6)	Dy(3)-O(56)	2.539(2)	Cl(6)-O(22)	1.435(3)

C(7)-C(8)	1.504(5)	O(55)-C(44)	1.439(4)	Cl(6)-O(23)	1.438(3)
C(9)-C(10)	1.529(5)	O(55)-C(37)	1.446(4)	Cl(7)-O(27)	1.404(4)
C(11)-C(12)	1.522(5)	O(56)-C(43)	1.443(4)	Cl(7)-O(26)	1.429(3)
C(15)-C(16)	1.526(5)	O(56)-C(42)	1.447(4)	Cl(7)-O(28)	1.436(3)
C(17)-C(18)	1.553(6)	O(57)-C(41)	1.456(4)	Cl(7)-O(25)	1.465(3)
C(57)-C(60)	1.461(6)	O(57)-C(40)	1.475(4)	Cl(8)-O(33)	1.437(2)
Dy(2)-O(53)	2.381(2)	O(58)-C(38)	1.441(4)	Cl(8)-O(36)	1.437(3)
Dy(2)-O(46)	2.387(2)	O(58)-C(39)	1.447(4)	Cl(8)-O(34)	1.439(3)
Dy(2)-O(51)	2.421(2)	O(59)-C(45)	1.443(4)	Cl(8)-O(35)	1.441(3)
Dy(2)-O(48)	2.424(2)	O(59)-C(54)	1.453(3)	Cl(9)-O(31)	1.434(3)
Dy(2)-O(52)	2.428(2)	O(60)-C(52)	1.445(3)	Cl(9)-O(32)	1.438(2)
Dy(2)-O(50)	2.433(2)	O(60)-C(53)	1.450(4)	Cl(9)-O(30)	1.440(3)
Dy(2)-O(54)	2.451(2)	O(61)-C(50)	1.444(4)	Cl(9)-O(29)	1.446(2)
Dy(2)-O(49)	2.461(2)	O(61)-C(51)	1.459(4)	N(3)-C(58)	1.138(5)
Dy(2)-O(47)	2.471(2)	O(62)-C(48)	1.441(4)	N(1)-C(55)	1.145(6)
O(46)-C(19)	1.448(4)	O(62)-C(49)	1.445(4)	C(59)-C(58)	1.451(6)
O(46)-C(25)	1.458(4)	O(63)-C(47)	1.445(4)	C(56)-C(55)	1.446(6)
O(47)-C(23)	1.441(4)				

Table S8, Angles (deg) for complex **4**

O(9)-Cl(3)-O(10)	109.01(16)	O(48)-Dy(2)-O(50)	98.94(8)	O(22)-Cl(6)-O(23)	109.8(2)
O(8)-Cl(2)-O(7)	112.54(19)	O(48)-Dy(2)-O(49)	92.75(8)	O(21)-Cl(6)-O(24)	108.8(3)
O(8)-Cl(2)-O(6)	108.44(17)	O(48)-Dy(2)-O(47)	136.31(7)	O(21)-Cl(6)-O(23)	108.93(17)
O(8)-Cl(2)-O(5)	109.5(2)	O(48)-C(22)-C(23)	109.4	O(21)-Cl(6)-O(22)	106.51(19)
O(63)-Dy(3)-O(62)	126.96(7)	O(48)-C(21)-C(26)	110.2	O(20)-Cl(5)-O(18)	110.70(16)
O(63)-Dy(3)-O(59)	63.75(7)	O(47)-C(24)-C(25)	110.3	O(2)-Cl(1)-O(4)	110.07(15)
O(63)-Dy(3)-O(58)	108.18(8)	O(47)-C(23)-C(22)	109.5	O(19)-Cl(5)-O(20)	110.01(16)
O(63)-Dy(3)-O(57)	65.89(7)	O(46)-Dy(2)-O(54)	167.07(7)	O(19)-Cl(5)-O(18)	111.8(2)
O(63)-Dy(3)-O(56)	110.02(7)	O(46)-Dy(2)-O(52)	119.93(7)	O(17)-Cl(5)-O(20)	108.93(15)
O(63)-Dy(3)-O(55)	131.14(7)	O(46)-Dy(2)-O(51)	177.7(5)	O(17)-Cl(5)-O(19)	109.68(16)
O(63)-C(47)-C(48)	109.9	O(46)-Dy(2)-O(50)	65.97(7)	O(17)-Cl(5)-O(18)	111.1(2)
O(63)-C(46)-C(45)	110.5	O(46)-Dy(2)-O(49)	123.01(7)	O(15)-Cl(4)-O(16)	109.05(17)
O(62)-Dy(3)-O(59)	65.79(7)	O(46)-Dy(2)-O(48)	125.74(8)	O(15)-Cl(4)-O(14)	108.52(16)
O(62)-Dy(3)-O(58)	81.34(7)	O(46)-Dy(2)-O(47)	123.90(7)	O(15)-Cl(4)-O(13)	108.89(17)
O(62)-Dy(3)-O(57)	142.02(7)	O(46)-C(25)-C(24)	110.3	O(14)-Cl(4)-O(16)	110.12(16)
O(62)-Dy(3)-O(56)	131.58(7)	O(46)-C(19)-H(19A)	119.78(18)	O(14)-Cl(4)-O(13)	108.60(17)
O(62)-Dy(3)-O(55)	68.91(7)	O(46)-C(19)-C(20)	111.4(2)	O(13)-Cl(4)-O(16)	109.02(19)
O(62)-C(49)-C(50)	110.5	O(45)-Dy(1)-O(44)	63.50(9)	O(12)-Cl(3)-O(9)	107.52(17)
O(62)-C(48)-C(47)	110.4	O(45)-Dy(1)-O(40)	123.44(9)	O(12)-Cl(3)-O(10)	111.11(18)
O(61)-Dy(3)-O(63)	108.6	O(45)-Dy(1)-O(39)	145.19(9)	O(11)-Cl(3)-O(9)	107.36(18)
O(61)-Dy(3)-O(62)	127.85(7)	O(45)-Dy(1)-O(38)	80.74(8)	O(11)-Cl(3)-O(12)	107.94(18)
O(61)-Dy(3)-O(59)	64.30(8)	O(45)-Dy(1)-O(37)	67.93(9)	O(11)-Cl(3)-O(10)	110.67(17)

O(61)-Dy(3)-O(58)	66.85(7)	O(45)-Dy(1)-N(2)	72.08(9)	O(1)-Cl(1)-O(4)	110.48(17)
O(61)-Dy(3)-O(57)	68.91(7)	O(45)-C(13)-C(14)	109.5	O(1)-Cl(1)-O(3)	110.3
O(61)-Dy(3)-O(56)	65.41(8)	O(45)-C(12)-C(11)	110.1	O(1)-Cl(1)-O(2)	110.3
O(61)-Dy(3)-O(55)	117.86(8)	O(44)-Dy(1)-O(40)	166.92(8)	N(3)-C(58)-C(59)	109.5
O(61)-C(51)-C(52)	110.6	O(44)-Dy(1)-O(39)	105.02(8)	N(2)-C(57)-C(60)	110.7
O(61)-C(50)-C(49)	110.5	O(44)-Dy(1)-O(38)	70.70(8)	N(1)-C(55)-C(56)	109.5
O(60)-Dy(3)-O(63)	110.4	O(44)-Dy(1)-O(37)	116.90(9)	C(9)-O(42)-Dy(1)	118.5(2)
O(60)-Dy(3)-O(62)	66.54(7)	O(44)-Dy(1)-N(2)	62.57(9)	C(9)-O(42)-C(18)	114.8(3)
O(60)-Dy(3)-O(61)	110.4	O(44)-C(15)-C(16)	110.5	C(8)-O(38)-Dy(1)	114.39(19)
O(60)-Dy(3)-O(59)	113.15(8)	O(44)-C(14)-C(13)	104.4(3)	C(8)-O(38)-C(1)	112.7(3)
O(60)-Dy(3)-O(58)	122.01(7)	O(43)-Dy(1)-O(45)	124.53(9)	C(7)-O(37)-Dy(1)	121.59(19)
O(60)-Dy(3)-O(57)	175.69(7)	O(43)-Dy(1)-O(44)	63.92(9)	C(6)-O(37)-Dy(1)	116.4(2)
O(60)-Dy(3)-O(56)	151.42(7)	O(43)-Dy(1)-O(41)	126.30(9)	C(6)-O(37)-C(7)	113.2(3)
O(60)-Dy(3)-O(55)	149.27(7)	O(43)-Dy(1)-O(40)	111.69(9)	C(57)-N(2)-Dy(1)	171.6(3)
O(60)-C(53)-C(54)	110.7	O(43)-Dy(1)-O(39)	66.39(9)	C(57)-C(60)-H(60B)	179.2(4)
O(60)-C(52)-C(51)	109.9	O(43)-Dy(1)-O(38)	97.69(8)	C(54)-O(59)-Dy(3)	115.06(19)
O(6)-Cl(2)-O(7)	110.29(18)	O(43)-Dy(1)-O(37)	157.37(8)	C(53)-O(60)-Dy(3)	120.78(17)
O(59)-Dy(3)-O(58)	69.27(8)	O(43)-Dy(1)-N(2)	69.29(9)	C(52)-O(60)-Dy(3)	119.50(17)
O(59)-Dy(3)-O(57)	84.17(7)	O(43)-C(17)-C(18)	110.3	C(52)-O(60)-C(53)	111.3(2)
O(59)-Dy(3)-O(56)	144.08(8)	O(43)-C(16)-C(15)	110.4	C(51)-O(61)-Dy(3)	119.39(17)
O(59)-Dy(3)-O(55)	119.85(7)	O(42)-Dy(1)-O(45)	129.69(9)	C(50)-O(61)-Dy(3)	120.74(17)
O(59)-C(54)-C(53)	109.8	O(42)-Dy(1)-O(44)	120.09(9)	C(50)-O(61)-C(51)	114.7(2)
O(59)-C(45)-C(46)	109.7	O(42)-Dy(1)-O(43)	67.60(9)	C(5)-O(40)-Dy(1)	121.0(2)
O(58)-Dy(3)-O(57)	88.78(7)	O(42)-Dy(1)-O(41)	68.28(9)	C(49)-O(62)-Dy(3)	115.83(18)
O(58)-Dy(3)-O(56)	70.91(7)	O(42)-Dy(1)-O(40)	65.59(9)	C(48)-O(62)-Dy(3)	123.64(19)
O(58)-Dy(3)-O(55)	111.95(7)	O(42)-Dy(1)-O(39)	84.97(9)	C(48)-O(62)-C(49)	113.8(2)
O(58)-C(39)-C(40)	110.6	O(42)-Dy(1)-O(38)	149.55(9)	C(47)-O(63)-Dy(3)	123.26(18)
O(58)-C(38)-C(37)	109.6	O(42)-Dy(1)-O(37)	121.46(9)	C(47)-O(63)-C(46)	113.4(2)
O(57)-Dy(3)-O(56)	93.11(7)	O(42)-Dy(1)-N(2)	68.94(9)	C(46)-O(63)-Dy(3)	117.65(19)
O(57)-C(41)-C(42)	110.1	O(42)-C(9)-C(10)	110	C(45)-O(59)-Dy(3)	119.72(18)
O(57)-C(40)-C(39)	109.9	O(42)-C(18)-C(17)	109.9	C(45)-O(59)-C(54)	113.9(2)
O(56)-C(43)-C(44)	110.3	O(41)-Dy(1)-O(45)	68.10(8)	C(44)-O(55)-Dy(3)	62.79(7)
O(56)-C(42)-C(41)	109.8	O(41)-Dy(1)-O(44)	117.96(9)	C(44)-O(55)-C(37)	82.32(7)
O(55)-Dy(3)-O(57)	70.88(8)	O(41)-Dy(1)-O(40)	74.85(8)	C(43)-O(56)-Dy(3)	115.43(17)
O(55)-Dy(3)-O(56)	114.82(8)	O(41)-Dy(1)-O(39)	136.44(8)	C(43)-O(56)-C(42)	116.2(2)
O(55)-C(44)-C(43)	110.6	O(41)-Dy(1)-O(38)	135.17(8)	C(42)-O(56)-Dy(3)	116.43(17)
O(55)-C(37)-H(37A)	122.04(18)	O(41)-Dy(1)-O(37)	74.68(8)	C(41)-O(57)-Dy(3)	122.90(17)
O(55)-C(37)-C(38)	111.2(2)	O(41)-Dy(1)-N(2)	67.40(9)	C(41)-O(57)-C(40)	111.7(2)
O(54)-Dy(2)-O(49)	66.13(7)	O(41)-C(11)-C(12)	110	C(40)-O(57)-Dy(3)	120.48(18)
O(54)-Dy(2)-O(47)	65.46(7)	O(41)-C(10)-C(9)	109.7	C(4)-O(40)-Dy(1)	113.6(2)
O(54)-C(36)-C(35)	110.4	O(40)-Dy(1)-N(2)	128.80(8)	C(4)-O(40)-C(5)	112.4(3)
O(54)-C(27)-C(28)	110.4	O(40)-C(4)-C(3)	108.9(3)	C(39)-O(58)-Dy(3)	119.91(18)
O(53)-Dy(2)-O(54)	65.05(7)	O(39)-Dy(1)-O(40)	62.71(8)	C(38)-O(58)-Dy(3)	110.67(17)

O(53)-Dy(2)-O(52)	71.13(7)	O(39)-Dy(1)-O(38)	64.58(8)	C(38)-O(58)-C(39)	111.9(2)
O(53)-Dy(2)-O(51)	108.8	O(39)-Dy(1)-O(37)	92.75(9)	C(37)-O(55)-Dy(3)	63.72(7)
O(53)-Dy(2)-O(50)	147.32(7)	O(39)-Dy(1)-N(2)	134.48(9)	C(36)-O(54)-Dy(2)	124.84(18)
O(53)-Dy(2)-O(49)	115.75(7)	O(39)-C(3)-C(4)	105.7(3)	C(36)-O(54)-C(27)	114.1(2)
O(53)-Dy(2)-O(48)	145.76(8)	O(39)-C(2)-C(1)	109.1(3)	C(35)-O(50)-Dy(2)	119.10(17)
O(53)-Dy(2)-O(47)	136.72(7)	O(38)-Dy(1)-O(40)	98.57(9)	C(34)-O(50)-Dy(2)	121.31(17)
O(53)-Dy(2)-O(46)	110.7	O(38)-Dy(1)-N(2)	132.59(8)	C(34)-O(50)-C(35)	111.4(2)
O(53)-C(29)-C(30)	110.9	O(38)-C(8)-C(7)	110.4	C(33)-O(51)-Dy(2)	118.82(18)
O(53)-C(28)-C(27)	110	O(38)-C(1)-C(2)	108.0(3)	C(33)-O(51)-C(32)	109.4(2)
O(52)-Dy(2)-O(54)	81.75(7)	O(37)-Dy(1)-O(40)	61.92(9)	C(32)-O(51)-Dy(2)	118.44(18)
O(52)-Dy(2)-O(50)	72.95(7)	O(37)-Dy(1)-O(38)	63.85(7)	C(31)-O(52)-Dy(2)	121.31(18)
O(52)-Dy(2)-O(49)	67.41(7)	O(37)-Dy(1)-N(2)	132.56(9)	C(31)-O(52)-C(30)	110.6(2)
O(52)-Dy(2)-O(47)	67.10(7)	O(37)-C(7)-C(8)	110.1	C(30)-O(52)-Dy(2)	111.92(18)
O(52)-C(31)-C(32)	110.3	O(36)-Cl(8)-O(35)	110.07(16)	C(3)-O(39)-Dy(1)	123.8(2)
O(52)-C(30)-C(29)	110.2	O(36)-Cl(8)-O(34)	107.96(18)	C(29)-O(53)-Dy(2)	120.63(18)
O(51)-Dy(2)-O(54)	97.16(7)	O(34)-Cl(8)-O(35)	109.05(18)	C(28)-O(53)-Dy(2)	121.47(18)
O(51)-Dy(2)-O(52)	113.49(7)	O(33)-Cl(8)-O(36)	112.4(3)	C(28)-O(53)-C(29)	111.2(2)
O(51)-Dy(2)-O(50)	71.40(7)	O(33)-Cl(8)-O(35)	108.83(16)	C(27)-O(54)-Dy(2)	120.65(18)
O(51)-Dy(2)-O(49)	64.92(7)	O(33)-Cl(8)-O(34)	106.70(18)	C(26)-O(49)-Dy(2)	115.13(17)
O(51)-Dy(2)-O(48)	81.86(7)	O(32)-Cl(9)-O(30)	109.42(17)	C(26)-O(49)-C(20)	117.0(2)
O(51)-Dy(2)-O(47)	71.40(7)	O(32)-Cl(9)-O(29)	110.1(2)	C(25)-O(46)-Dy(2)	74.48(7)
O(51)-C(33)-C(34)	110	O(31)-Cl(9)-O(32)	109.38(16)	C(24)-O(47)-Dy(2)	113.99(17)
O(51)-C(32)-C(31)	110.6	O(31)-Cl(9)-O(30)	110.1(2)	C(23)-O(47)-Dy(2)	114.13(17)
O(50)-Dy(2)-O(54)	129.91(7)	O(31)-Cl(9)-O(29)	109.39(17)	C(23)-O(47)-C(24)	117.0(2)
O(50)-Dy(2)-O(49)	140.27(7)	O(30)-Cl(9)-O(29)	108.44(17)	C(22)-O(48)-Dy(2)	121.89(17)
O(50)-Dy(2)-O(47)	70.55(7)	O(3)-Cl(1)-O(4)	109.75(17)	C(22)-O(48)-C(21)	111.8(2)
O(50)-C(35)-C(36)	110.3	O(3)-Cl(1)-O(2)	108.6	C(21)-O(48)-Dy(2)	119.60(17)
O(50)-C(34)-C(33)	110.4	O(28)-Cl(7)-O(25)	110.18(17)	C(20)-O(49)-Dy(2)	114.18(17)
O(5)-Cl(2)-O(7)	110.98(17)	O(27)-Cl(7)-O(28)	109.89(16)	C(2)-O(39)-Dy(1)	112.7(2)
O(5)-Cl(2)-O(6)	108.60(17)	O(27)-Cl(7)-O(26)	108.86(18)	C(2)-O(39)-C(3)	113.5(3)
O(49)-Dy(2)-O(47)	95.51(7)	O(27)-Cl(7)-O(25)	108.6(2)	C(19)-O(46)-Dy(2)	140.53(7)
O(49)-C(26)-C(21)	109.3	O(26)-Cl(7)-O(28)	108.83(17)	C(19)-O(46)-C(25)	123.09(7)
O(49)-C(20)-C(19)	109.3	O(26)-Cl(7)-O(25)	110.91(19)	C(18)-O(42)-Dy(1)	121.3(2)
O(48)-Dy(2)-O(54)	65.14(7)	O(24)-Cl(6)-O(23)	110.5(2)	C(17)-O(43)-Dy(1)	116.5(2)
O(48)-Dy(2)-O(52)	65.40(7)	O(24)-Cl(6)-O(22)	107.79(17)	C(16)-O(43)-Dy(1)	124.1(2)
C(16)-O(43)-C(17)	114.6(3)	C(13)-O(45)-Dy(1)	121.7(2)	C(11)-O(41)-C(10)	107.9(3)
C(15)-O(44)-Dy(1)	120.2(2)	C(13)-O(45)-C(12)	113.7(3)	C(10)-O(41)-Dy(1)	118.3(2)
C(15)-O(44)-C(14)	115.3(3)	C(12)-O(45)-Dy(1)	115.2(2)	C(1)-O(38)-Dy(1)	119.5(2)
C(14)-O(44)-Dy(1)	120.7(2)	C(11)-O(41)-Dy(1)	118.6(2)		

Table S9, Bond lengths (Å) for complex **5**

Dy(1)-O(8)	2.419(6)	Dy(1)-N(2)	2.863(5)	C(1)-C(2)	1.342(12)

Dy(1)-O(7)	2.420(6)	Cl(1)-O(10)	1.368(8)	C(1)-O(1)	1.440(8)
Dy(1)-O(5)	2.431(3)	Cl(1)-O(11)#1	1.371(8)	C(2)-O(2)	1.409(9)
Dy(1)-O(5)#1	2.431(3)	Cl(1)-O(11)	1.371(8)	C(3)-C(4)	1.370(10)
Dy(1)-O(4)	2.450(5)	Cl(1)-O(12)	1.405(9)	C(3)-O(2)	1.383(8)
Dy(1)-O(1)	2.455(5)	N(1)-O(6)	1.221(8)	C(4)-O(3)	1.369(7)
Dy(1)-O(2)#1	2.499(4)	N(1)-O(5)	1.263(5)	C(5)-C(6)	1.390(10)
Dy(1)-O(2)	2.499(4)	N(1)-O(5)#1	1.263(5)	C(5)-O(3)	1.423(8)
Dy(1)-O(3)	2.503(4)	N(2)-O(8)	1.206(8)	C(6)-O(4)	1.424(7)
Dy(1)-O(3)#1	2.503(4)	N(2)-O(9)	1.212(7)	O(1)-C(1)#1	1.440(8)
Dy(1)-N(1)	2.843(6)	N(2)-O(7)	1.217(7)	O(4)-C(6)#1	1.424(7)

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

Table S10, Angles (deg) for complex **5**

O(8)-Dy(1)-O(7)	49.47(19)	O(2)-Dy(1)-O(3)	60.75(14)	O(11)#1-Cl(1)-O(12)	110.3(5)
O(8)-Dy(1)-O(5)	143.17(13)	O(8)-Dy(1)-O(3)#1	70.26(15)	O(11)-Cl(1)-O(12)	110.3(5)
O(7)-Dy(1)-O(5)	145.92(12)	O(7)-Dy(1)-O(3)#1	94.78(15)	O(6)-N(1)-O(5)	121.8(3)
O(8)-Dy(1)-O(5)#1	143.17(13)	O(5)-Dy(1)-O(3)#1	119.04(16)	O(6)-N(1)-O(5)#1	121.8(3)
O(7)-Dy(1)-O(5)#1	145.92(13)	O(5)#1-Dy(1)-O(3)#1	74.47(17)	O(5)-N(1)-O(5)#1	116.4(5)
O(5)-Dy(1)-O(5)#1	52.41(17)	O(4)-Dy(1)-O(3)#1	63.21(10)	O(6)-N(1)-Dy(1)	174.9(6)
O(8)-Dy(1)-O(4)	80.0(2)	O(1)-Dy(1)-O(3)#1	121.48(10)	O(5)-N(1)-Dy(1)	58.4(3)
O(7)-Dy(1)-O(4)	129.51(19)	O(2)#1-Dy(1)-O(3)#1	60.74(14)	O(5)#1-N(1)-Dy(1)	58.4(3)
O(5)-Dy(1)-O(4)	74.88(16)	O(2)-Dy(1)-O(3)#1	164.5(2)	O(8)-N(2)-O(9)	122.8(6)
O(5)#1-Dy(1)-O(4)	74.88(16)	O(3)-Dy(1)-O(3)#1	117.0(2)	O(8)-N(2)-O(7)	113.3(6)
O(8)-Dy(1)-O(1)	130.6(2)	O(8)-Dy(1)-N(1)	151.5(2)	O(9)-N(2)-O(7)	123.9(6)
O(7)-Dy(1)-O(1)	81.2(2)	O(7)-Dy(1)-N(1)	159.01(19)	O(8)-N(2)-Dy(1)	56.6(4)
O(5)-Dy(1)-O(1)	77.68(16)	O(5)-Dy(1)-N(1)	26.25(9)	O(9)-N(2)-Dy(1)	179.4(4)
O(5)#1-Dy(1)-O(1)	77.68(16)	O(5)#1-Dy(1)-N(1)	26.25(9)	O(7)-N(2)-Dy(1)	56.7(3)
O(4)-Dy(1)-O(1)	149.3(2)	O(4)-Dy(1)-N(1)	71.48(19)	C(2)-C(1)-O(1)	113.0(6)
O(8)-Dy(1)-O(2)#1	95.48(16)	O(1)-Dy(1)-N(1)	77.86(19)	C(1)-C(2)-O(2)	111.4(9)
O(7)-Dy(1)-O(2)#1	70.75(15)	O(2)#1-Dy(1)-N(1)	99.31(16)	C(4)-C(3)-O(2)	113.4(6)
O(5)-Dy(1)-O(2)#1	120.57(17)	O(2)-Dy(1)-N(1)	99.31(16)	O(3)-C(4)-C(3)	114.0(6)
O(5)#1-Dy(1)-O(2)#1	75.90(17)	O(3)-Dy(1)-N(1)	96.14(16)	C(6)-C(5)-O(3)	110.3(6)
O(4)-Dy(1)-O(2)#1	121.61(10)	O(3)#1-Dy(1)-N(1)	96.14(16)	C(5)-C(6)-O(4)	111.7(6)
O(1)-Dy(1)-O(2)#1	63.04(12)	O(8)-Dy(1)-N(2)	24.59(18)	C(1)-O(1)-C(1)#1	119.0(9)
O(8)-Dy(1)-O(2)	95.49(17)	O(7)-Dy(1)-N(2)	24.88(17)	C(1)-O(1)-Dy(1)	119.6(4)
O(7)-Dy(1)-O(2)	70.75(15)	O(5)-Dy(1)-N(2)	153.70(9)	C(1)#1-O(1)-Dy(1)	119.6(4)
O(5)-Dy(1)-O(2)	75.90(17)	O(5)#1-Dy(1)-N(2)	153.70(9)	C(3)-O(2)-C(2)	116.2(6)
O(5)#1-Dy(1)-O(2)	120.56(17)	O(4)-Dy(1)-N(2)	104.63(18)	C(3)-O(2)-Dy(1)	124.0(4)
O(4)-Dy(1)-O(2)	121.61(10)	O(1)-Dy(1)-N(2)	106.03(19)	C(2)-O(2)-Dy(1)	119.6(5)
O(1)-Dy(1)-O(2)	63.04(12)	O(2)#1-Dy(1)-N(2)	82.67(16)	C(4)-O(3)-C(5)	117.2(5)
O(2)#1-Dy(1)-O(2)	116.8(2)	O(2)-Dy(1)-N(2)	82.67(16)	C(4)-O(3)-Dy(1)	122.9(4)
O(8)-Dy(1)-O(3)	70.26(15)	O(3)-Dy(1)-N(2)	81.88(15)	C(5)-O(3)-Dy(1)	119.4(4)
O(7)-Dy(1)-O(3)	94.78(15)	O(3)#1-Dy(1)-N(2)	81.88(15)	C(6)#1-O(4)-C(6)	117.7(7)

O(5)-Dy(1)-O(3)	74.47(17)	N(1)-Dy(1)-N(2)	176.11(17)	C(6)#1-O(4)-Dy(1)	120.7(3)
O(5)#1-Dy(1)-O(3)	119.04(16)	O(10)-Cl(1)-O(11)#1	110.7(5)	C(6)-O(4)-Dy(1)	120.7(3)
O(4)-Dy(1)-O(3)	63.21(10)	O(10)-Cl(1)-O(11)	110.7(5)	N(1)-O(5)-Dy(1)	95.4(3)
O(1)-Dy(1)-O(3)	121.48(10)	O(11)#1-Cl(1)-O(11)	102.0(10)	N(2)-O(7)-Dy(1)	98.4(4)
O(2)#1-Dy(1)-O(3)	164.5(2)	O(10)-Cl(1)-O(12)	112.3(6)	N(2)-O(8)-Dy(1)	98.8(4)

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

Table S11, Bond lengths (Å) for complex **6**

Dy(1)-O(5)	2.402(3)	O(12)-C(11)	1.434(5)	C(18)-C(13)	1.404(7)
Dy(1)-O(1)	2.412(3)	O(12)-C(10)	1.449(6)	C(18)-B(1)	1.648(7)
Dy(1)-O(4)	2.431(3)	O(8)-C(2)	1.429(7)	C(29)-C(30)	1.393(7)
Dy(1)-O(2)	2.439(3)	O(8)-C(3)	1.437(6)	C(19)-C(20)	1.388(7)
Dy(1)-O(12)	2.449(3)	O(9)-C(4)	1.450(6)	C(26)-C(25)	1.409(6)
Dy(1)-O(9)	2.478(3)	O(9)-C(5)	1.455(7)	C(23)-C(22)	1.403(7)
Dy(1)-O(7)	2.487(3)	O(10)-C(6)	1.424(8)	C(13)-C(14)	1.393(7)
Dy(1)-O(10)	2.515(3)	O(10)-C(7)	1.445(6)	C(14)-C(15)	1.385(8)
Dy(1)-O(8)	2.549(3)	C(10)-C(9)	1.500(7)	C(15)-C(16)	1.380(8)
Dy(1)-O(11)	2.562(3)	C(2)-C(1)	1.486(8)	C(22)-C(21)	1.382(9)
Dy(1)-N(1)	2.847(4)	C(6)-C(5)	1.302(10)	C(21)-C(20)	1.380(9)
Dy(1)-N(2)	2.855(4)	C(8)-C(7)	1.484(8)	C(25)-C(30)	1.416(6)
N(2)-O(6)	1.213(5)	C(4)-C(3)	1.472(8)	C(25)-B(1)	1.653(7)
N(2)-O(5)	1.275(5)	C(27)-C(28)	1.370(7)	C(31)-C(32)	1.403(7)
N(2)-O(4)	1.283(5)	C(27)-C(26)	1.392(6)	C(31)-C(36)	1.411(6)
N(1)-O(3)	1.220(5)	C(28)-C(29)	1.404(7)	C(31)-B(1)	1.661(7)
N(1)-O(2)	1.273(5)	C(17)-C(16)	1.397(7)	C(34)-C(35)	1.378(8)
N(1)-O(1)	1.277(5)	C(17)-C(18)	1.399(7)	C(34)-C(33)	1.391(8)
O(11)-C(9)	1.426(6)	C(24)-C(23)	1.403(7)	C(32)-C(33)	1.390(7)
O(11)-C(8)	1.431(6)	C(24)-C(19)	1.415(7)	C(36)-C(35)	1.391(6)
O(7)-C(1)	1.434(6)	C(24)-B(1)	1.636(7)	C(12)-C(11)	1.495(7)
O(7)-C(12)	1.456(6)				

Table S12, Angles (deg) for complex **6**

O(5)-Dy(1)-O(1)	149.86(12)	O(9)-Dy(1)-N(1)	72.00(12)	O(12)-C(10)-C(9)	106.9(4)
O(5)-Dy(1)-O(4)	52.88(11)	O(7)-Dy(1)-N(1)	105.97(11)	O(8)-C(2)-C(1)	104.7(4)
O(1)-Dy(1)-O(4)	137.30(12)	O(10)-Dy(1)-N(1)	103.86(13)	O(11)-C(9)-C(10)	105.1(4)
O(5)-Dy(1)-O(2)	136.30(12)	O(8)-Dy(1)-N(1)	89.53(12)	C(5)-C(6)-O(10)	115.4(7)
O(1)-Dy(1)-O(2)	52.91(11)	O(11)-Dy(1)-N(1)	91.66(11)	O(11)-C(8)-C(7)	105.5(4)
O(4)-Dy(1)-O(2)	152.01(12)	O(5)-Dy(1)-N(2)	26.31(11)	O(10)-C(7)-C(8)	106.7(4)
O(5)-Dy(1)-O(12)	130.20(12)	O(1)-Dy(1)-N(2)	153.70(11)	O(9)-C(4)-C(3)	106.6(4)
O(1)-Dy(1)-O(12)	77.94(12)	O(4)-Dy(1)-N(2)	26.57(11)	C(6)-C(5)-O(9)	113.2(6)
O(4)-Dy(1)-O(12)	83.21(12)	O(2)-Dy(1)-N(2)	153.33(12)	O(8)-C(3)-C(4)	106.4(4)
O(2)-Dy(1)-O(12)	73.72(11)	O(12)-Dy(1)-N(2)	107.07(12)	O(7)-C(1)-C(2)	109.0(4)
O(5)-Dy(1)-O(9)	82.11(13)	O(9)-Dy(1)-N(2)	106.16(13)	C(28)-C(27)-C(26)	120.8(5)

O(1)-Dy(1)-O(9)	72.66(13)	O(7)-Dy(1)-N(2)	74.74(11)	C(27)-C(28)-C(29)	119.1(4)
O(4)-Dy(1)-O(9)	129.36(12)	O(10)-Dy(1)-N(2)	75.44(13)	C(16)-C(17)-C(18)	123.1(5)
O(2)-Dy(1)-O(9)	76.31(12)	O(8)-Dy(1)-N(2)	89.29(12)	C(23)-C(24)-C(19)	115.4(4)
O(12)-Dy(1)-O(9)	146.76(13)	O(11)-Dy(1)-N(2)	89.53(11)	C(23)-C(24)-B(1)	121.4(4)
O(5)-Dy(1)-O(7)	79.91(12)	N(1)-Dy(1)-N(2)	178.14(12)	C(19)-C(24)-B(1)	122.4(4)
O(1)-Dy(1)-O(7)	128.25(11)	O(6)-N(2)-O(5)	122.6(4)	C(17)-C(18)-C(13)	114.7(4)
O(4)-Dy(1)-O(7)	73.44(12)	O(6)-N(2)-O(4)	122.8(4)	C(17)-C(18)-B(1)	124.6(4)
O(2)-Dy(1)-O(7)	82.25(11)	O(5)-N(2)-O(4)	114.6(4)	C(13)-C(18)-B(1)	120.7(4)
O(12)-Dy(1)-O(7)	64.27(11)	O(6)-N(2)-Dy(1)	177.6(3)	C(30)-C(29)-C(28)	119.5(4)
O(9)-Dy(1)-O(7)	125.18(11)	O(5)-N(2)-Dy(1)	56.6(2)	C(20)-C(19)-C(24)	122.4(5)
O(5)-Dy(1)-O(10)	73.77(13)	O(4)-N(2)-Dy(1)	58.0(2)	C(27)-C(26)-C(25)	122.8(4)
O(1)-Dy(1)-O(10)	80.67(12)	O(3)-N(1)-O(2)	122.1(4)	C(24)-C(23)-C(22)	122.3(5)
O(4)-Dy(1)-O(10)	79.52(12)	O(3)-N(1)-O(1)	122.0(4)	C(14)-C(13)-C(18)	123.0(5)
O(2)-Dy(1)-O(10)	126.83(11)	O(2)-N(1)-O(1)	115.9(4)	C(15)-C(14)-C(13)	120.0(5)
O(12)-Dy(1)-O(10)	125.07(10)	O(3)-N(1)-Dy(1)	177.1(3)	C(16)-C(15)-C(14)	119.0(5)
O(9)-Dy(1)-O(10)	65.03(11)	O(2)-N(1)-Dy(1)	58.6(2)	C(21)-C(22)-C(23)	120.2(5)
O(7)-Dy(1)-O(10)	150.17(12)	O(1)-N(1)-Dy(1)	57.4(2)	C(15)-C(16)-C(17)	120.0(5)
O(5)-Dy(1)-O(8)	68.38(12)	C(9)-O(11)-C(8)	114.1(4)	C(20)-C(21)-C(22)	119.3(5)
O(1)-Dy(1)-O(8)	111.81(11)	C(9)-O(11)-Dy(1)	117.6(3)	C(26)-C(25)-C(30)	114.6(4)
O(4)-Dy(1)-O(8)	110.90(12)	C(8)-O(11)-Dy(1)	118.0(3)	C(26)-C(25)-B(1)	121.9(4)
O(2)-Dy(1)-O(8)	67.97(12)	N(2)-O(5)-Dy(1)	97.1(3)	C(30)-C(25)-B(1)	123.4(4)
O(12)-Dy(1)-O(8)	117.10(11)	C(1)-O(7)-C(12)	112.9(4)	C(21)-C(20)-C(19)	120.5(5)
O(9)-Dy(1)-O(8)	62.45(12)	C(1)-O(7)-Dy(1)	118.2(3)	C(32)-C(31)-C(36)	114.7(4)
O(7)-Dy(1)-O(8)	62.76(11)	C(12)-O(7)-Dy(1)	112.8(3)	C(32)-C(31)-B(1)	122.9(4)
O(10)-Dy(1)-O(8)	117.79(11)	N(1)-O(2)-Dy(1)	95.0(2)	C(36)-C(31)-B(1)	122.0(4)
O(5)-Dy(1)-O(11)	110.55(11)	C(11)-O(12)-C(10)	113.5(3)	C(35)-C(34)-C(33)	119.1(5)
O(1)-Dy(1)-O(11)	69.40(11)	C(11)-O(12)-Dy(1)	121.1(3)	C(33)-C(32)-C(31)	123.2(5)
O(4)-Dy(1)-O(11)	67.90(12)	C(10)-O(12)-Dy(1)	120.9(3)	C(32)-C(33)-C(34)	119.8(5)
O(2)-Dy(1)-O(11)	113.11(11)	C(2)-O(8)-C(3)	112.3(4)	C(35)-C(36)-C(31)	122.8(4)
O(12)-Dy(1)-O(11)	63.05(10)	C(2)-O(8)-Dy(1)	120.4(3)	C(24)-B(1)-C(18)	111.1(4)
O(9)-Dy(1)-O(11)	118.16(12)	C(3)-O(8)-Dy(1)	116.8(3)	C(24)-B(1)-C(25)	107.1(4)
O(7)-Dy(1)-O(11)	116.66(11)	N(1)-O(1)-Dy(1)	96.1(2)	C(18)-B(1)-C(25)	111.6(4)
O(10)-Dy(1)-O(11)	62.10(11)	N(2)-O(4)-Dy(1)	95.5(3)	C(24)-B(1)-C(31)	112.0(4)
O(8)-Dy(1)-O(11)	178.79(12)	C(4)-O(9)-C(5)	114.7(5)	C(18)-B(1)-C(31)	104.9(3)
O(5)-Dy(1)-N(1)	151.88(11)	C(4)-O(9)-Dy(1)	122.2(3)	C(25)-B(1)-C(31)	110.4(4)
O(1)-Dy(1)-N(1)	26.49(11)	C(5)-O(9)-Dy(1)	116.0(4)	C(29)-C(30)-C(25)	123.1(4)
O(4)-Dy(1)-N(1)	155.22(11)	C(6)-O(10)-C(7)	113.9(5)	C(34)-C(35)-C(36)	120.3(5)
O(2)-Dy(1)-N(1)	26.44(11)	C(6)-O(10)-Dy(1)	115.3(3)	O(7)-C(12)-C(11)	105.0(4)
O(12)-Dy(1)-N(1)	74.76(11)	C(7)-O(10)-Dy(1)	120.5(3)	O(12)-C(11)-C(12)	105.9(4)

2 SHAPE parameters

Table S13, Continuous Shape Measures calculation for complexes **1-6**

Structure	DP-10	EPY-10	OBPY-10	PPR-10	PAPR-10	JBCCU-10	JBCSAPR-10	JMBIC-10	JATDI-10	JSPC-10	SDD-10	TD-10	HD-10
1	36.068	23.383	14.628	11.171	11.791	11.072	4.456	7.396	18.564	2.837	4.115	3.236	7.979
	EP-9	OPY-9	HBPY-9	JTC-9	JCCU-9	CCU-9	JCSAPR-9	CSAPR-9	JTCTPR-9	TCTPR-9	JTDIC-9	HH-9	MFF-9
2	35.05	21.641	16.159	15.852	10.638	9.215	3.018	1.952	4.502	1.714	12.083	9.919	1.597
	OP-8	HPY-8	HBPY-8	CU-8	SAPR-8	TDD-8	JGBF-8	JETBPY-8	JBTPR-8	BTPR-8	JSD-8	TT-8	ETBPY-8
3	32.132	22.548	16.025	8.895	0.822	2.337	16.222	29.684	2.575	1.942	5.312	9.495	24.59
	EP-9	OPY-9	HBPY-9	JTC-9	JCCU-9	CCU-9	JCSAPR-9	CSAPR-9	JTCTPR-9	TCTPR-9	JTDIC-9	HH-9	MFF-9
4-9-1	35.544	24.691	13.992	14.481	8.104	6.743	3.992	3.044	4.73	3.492	10.425	9.609	2.231
4-9-2	32.499	24.216	13.388	13.709	6.377	5.104	6.359	5.486	7.08	6.537	9.724	7.864	4.56
	DP-10	EPY-10	OBPY-10	PPR-10	PAPR-10	JBCCU-10	JBCSAPR-10	JMBIC-10	JATDI-10	JSPC-10	SDD-10	TD-10	HD-10
4-10	37.429	23.595	16.074	10.411	14.526	13.653	4.226	10.217	17.494	1.638	6.301	5.082	11.48
	DP-10	EPY-10	OBPY-10	PPR-10	PAPR-10	JBCCU-10	JBCSAPR-10	JMBIC-10	JATDI-10	JSPC-10	SDD-10	TD-10	HD-10
5	37.316	26.366	15.196	11.677	12.068	10.674	5.542	8	19.671	2.286	3.511	2.429	7.547
	DP-10	EPY-10	OBPY-10	PPR-10	PAPR-10	JBCCU-10	JBCSAPR-10	JMBIC-10	JATDI-10	JSPC-10	SDD-10	TD-10	HD-10
6	36.26	24.843	14.753	12.87	11.863	8.778	3.101	7.235	20.482	3.408	4.921	3.949	6.184

DP-10 D_{10h} Decagon; EPY-10 C_{9v} Enneagonal pyramid; OBPY-10 D_{8h} Octagonal bipyramid; PPR-10 D_{5h};Pentagonal prism; PAPR-10 D_{5d} Pentagonal antiprism; JBCCU-10 D_{4h} Bicapped cube J15; JBCSAPR-10 D_{4d} Bicapped square antiprism J17; JMBIC-10 C_{2v} Metabidiminished icosahedron J62; JATDI-10 C_{3v} Augmented tridiminished icosahedron J_{64}; JSPC-10 C2v Sphenocorona; SDD-10 D_2 Staggered Dodecahedron (2:6:2); TD-10 C_{2v} Tetradecahedron (2:6:2); HD-10 D_{4h} Hexadecahedron (2:6:2) or (1:4:4:1)

EP-9 D_{9h} Enneagon; OPY-9 C_{8v} Octagonal pyramid; HBPY-9 D_{7h} Heptagonal bipyramid; JTC-9 C_{3v} Johnson triangular cupola J3; JCCU-9 C_{4v} Capped cube J8; CCU-9 C_{4v} Spherical-relaxed capped cube; JCSAPR-9 C_{4v} Capped square antiprism J10; CSAPR-9 C_{4v} Spherical capped square antiprism; JTCTPR-9 D_{3h} Tricapped trigonal prism J51; TCTPR-9 D_{3h} Spherical tricapped trigonal prism; JTDIC-9 C_{3v} Tridiminished icosahedron J63; HH-9 C_{2v} Hula-hoop; MFF-9 C_s Muffin

OP-8 D_{8h} Octagon; HPY-8 C_{7v} Heptagonal pyramid; HBPY-8 D_{6h} Hexagonal bipyramid; CU-8 O_h Cube; SAPR-8 D_{4d} Square antiprism; TDD-8 D_{2d} Triangular dodecahedron; JGBF-8 D_{2d} Johnson gyrobifastigium J26; JETBPY-8 D_{3h} Johnson elongated triangular bipyramid J14; JBTPR-8 C_{2v} Biaugmented trigonal prism J50; BTPR-8 C_{2v} Biaugmented trigonal prism; JSD-8 D_{2d} Snub diphenoid J84; TT-8 T_d Triakis tetrahedron; ETBPY-8 D_{3h} Elongated trigonal bipyramid

4-9-1, 4-9-2, 4-10: the 9-coordinate and 10-coordinated parts for complex **4**

3. Powder X-ray diffraction

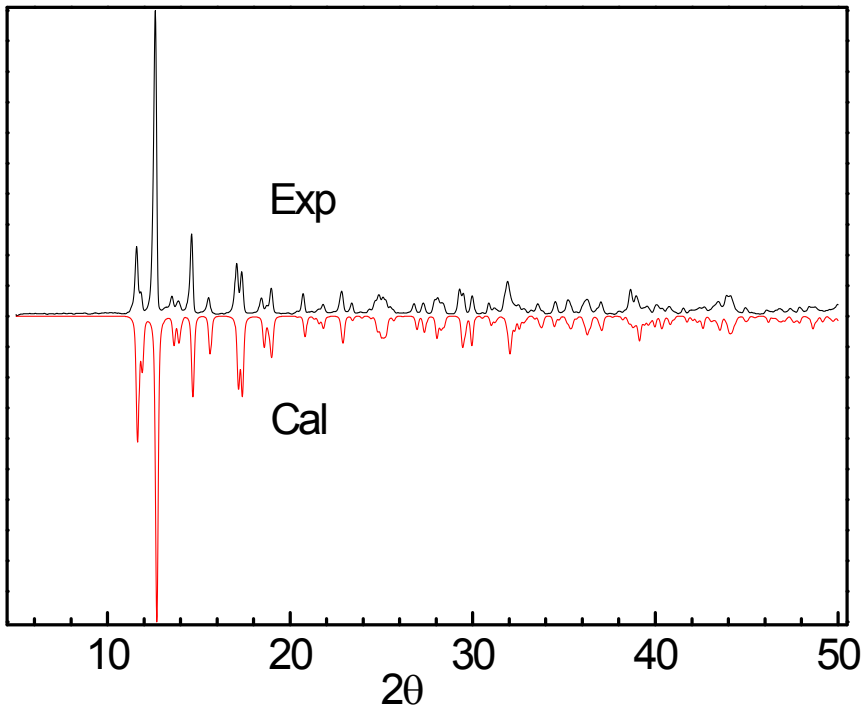

Fig S1 PXRD patterns for complex **1**

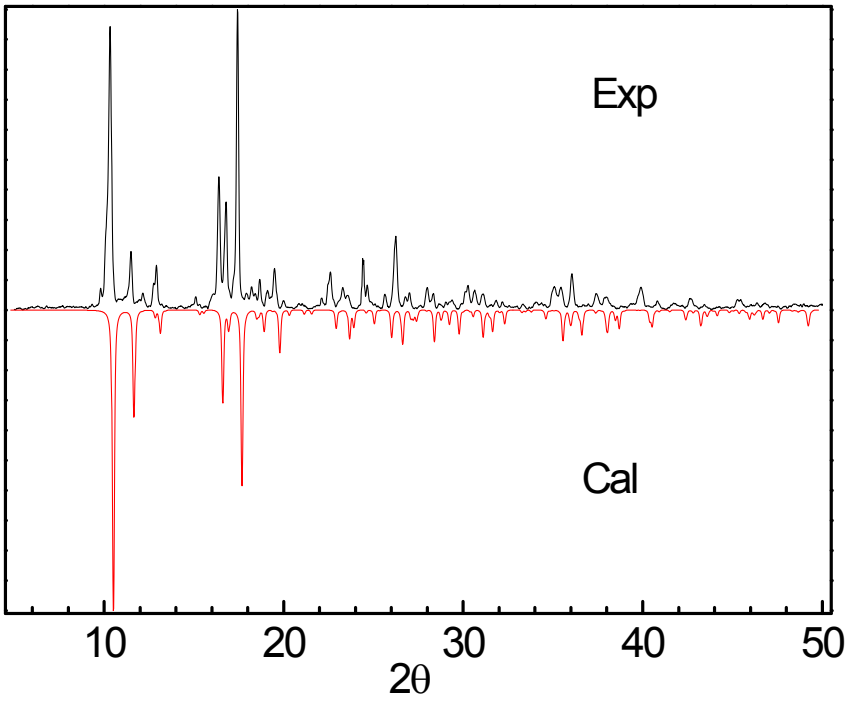

Fig S2 PXRD patterns for complex **2**

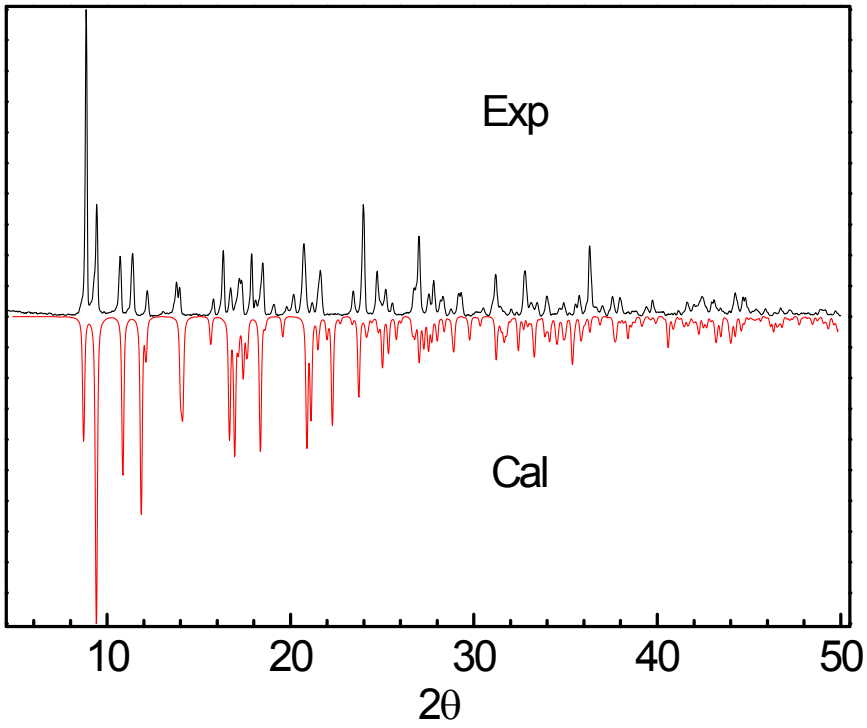

Fig S3 PXRD patterns for complex **3**

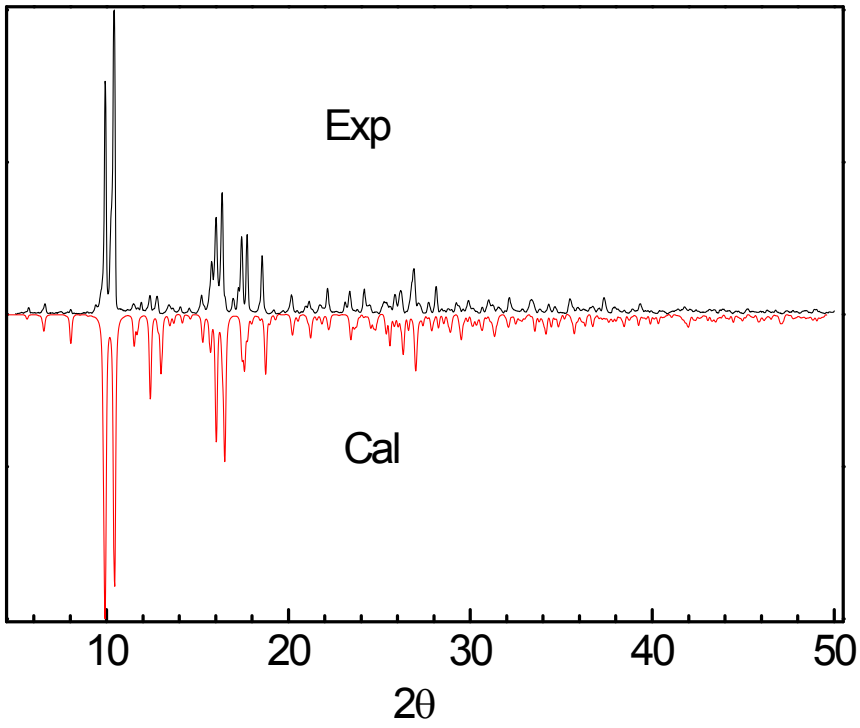

Fig S4 PXRD patterns for complex **4**

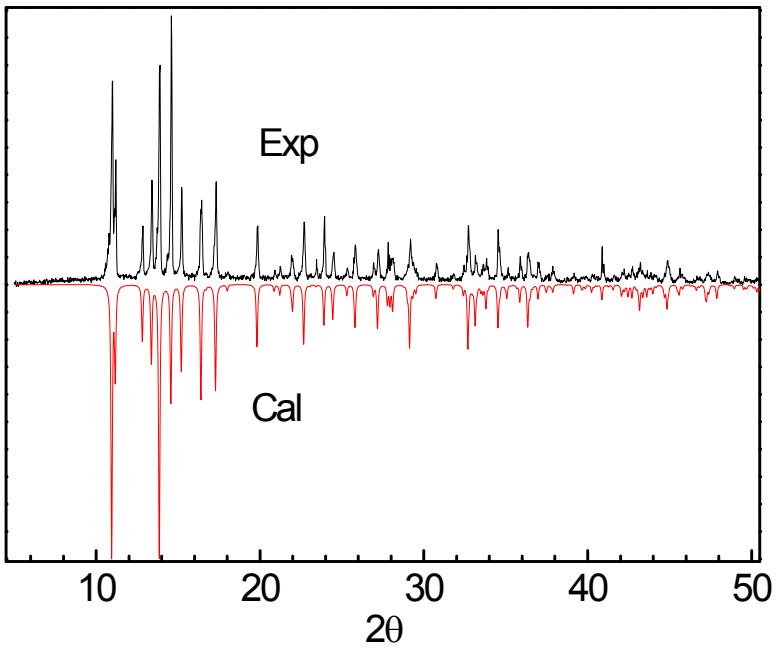

Fig S5 PXRD patterns for complex **5**

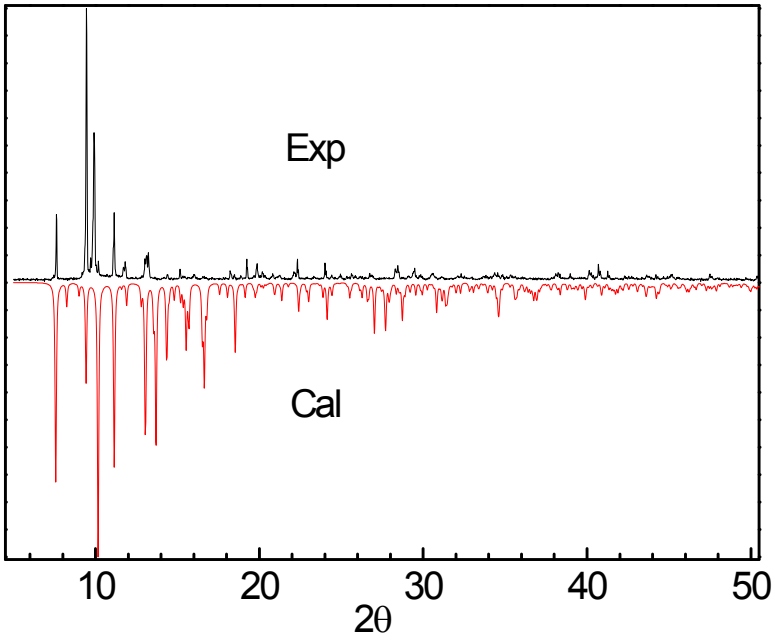

Fig S6 PXRD patterns for complex **6**

4. Magnetic data

4.1 Magnetic data for complex 1

Table S14: Relaxation Fitting Parameters of a generalized Debye model for **1**.

T	χ_S	χ_T	τ	α
2	0.88453	3.81735	0.00791	0.42057
2.4	0.79836	3.45928	0.00511	0.32478
2.8	0.72836	3.25982	0.00398	0.25599
3.2	0.67257	3.02975	0.00301	0.20241
3.6	0.62332	2.81703	0.00227	0.1685
4	0.57928	2.58988	0.00151	0.13071
4.4	0.53128	2.38029	8.23E-04	0.10026
4.8	0.49335	2.19763	3.60E-04	0.06665
5.2	0.45105	2.04966	1.35E-04	0.05303
5.6	0.23487	1.91935	4.22E-05	0.07647
6	3.10E-14	1.79954	1.30E-05	0.09373

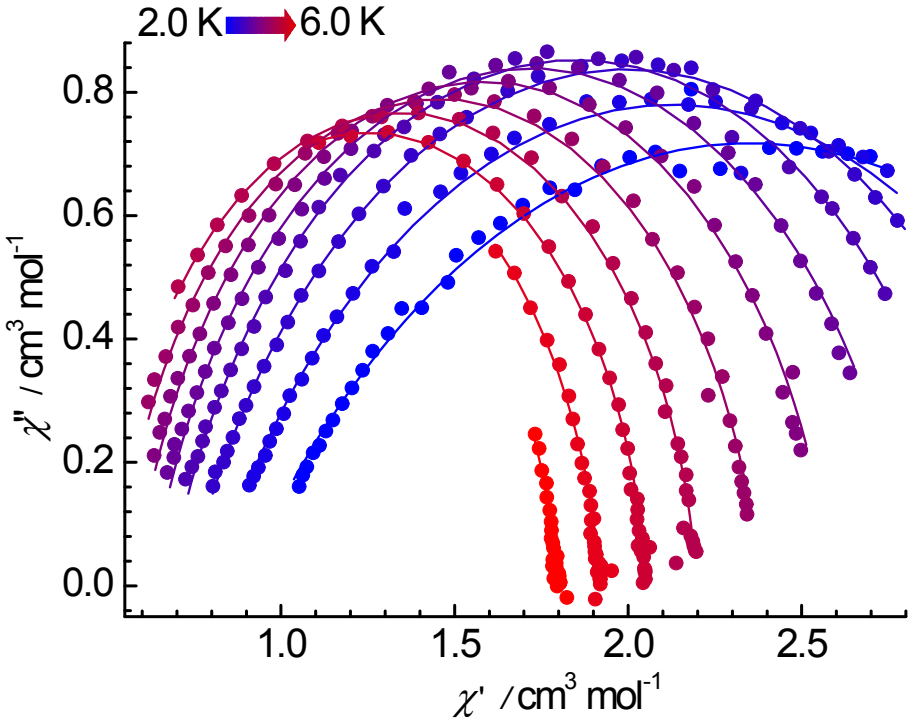

Fig S7 Cole-Cole plots using the frequency-dependence ac susceptibility data under a dc field of 1000 Oe for **1**. The solid lines are the best fits.

4.2 Magnetic data for complex 2

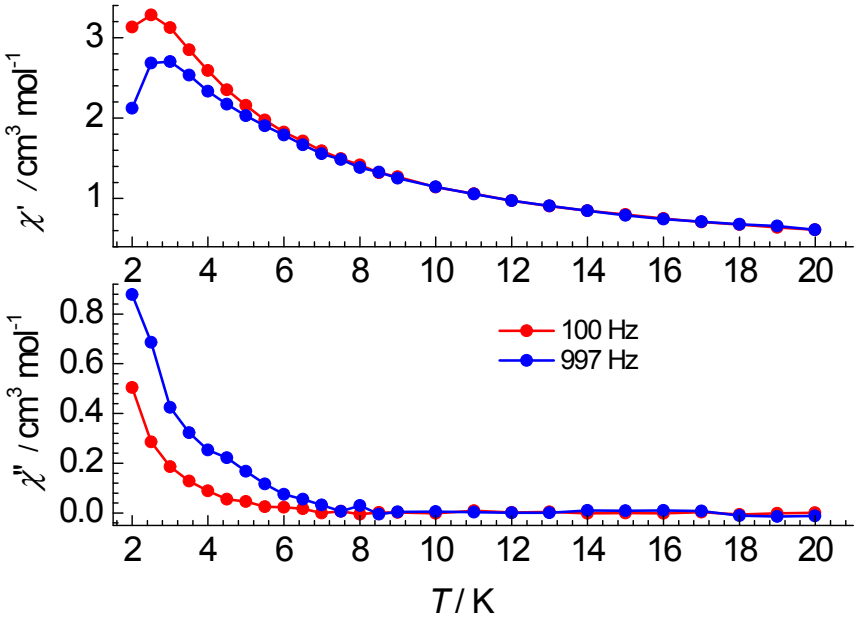

Fig S8. Temperature-dependence of the in-phase (χ', top) and out-of-phase (χ'', bottom) ac susceptibility signals under a dc field of 1000 Oe at the indicated frequencies for **2**, only a small tail is observed.

4.3 Magnetic data for complex 3

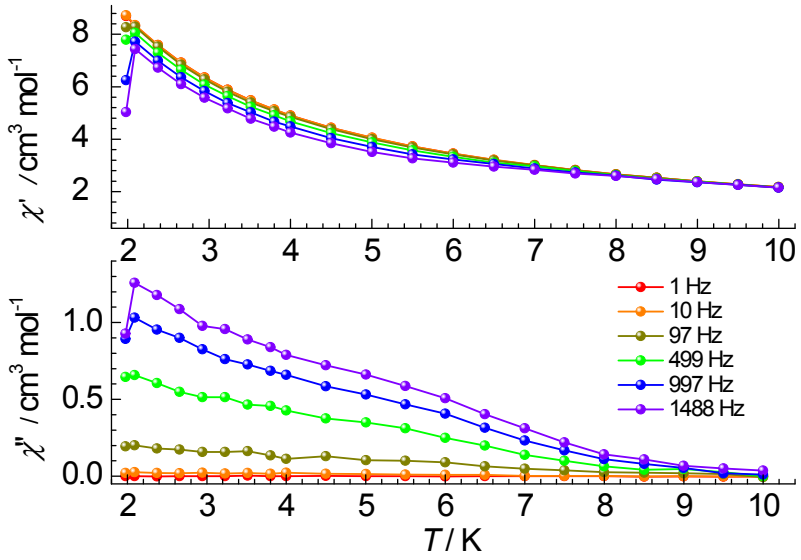

Fig S9. Temperature-dependence of the in-phase (χ') and out-of-phase (χ'',) ac susceptibility signals under a zero dc field at the indicated frequencies for **3**.

Table S15: Relaxation Fitting Parameters of a generalized Debye model for **3** (1000 Oe).

T	χ_S	χ_T	τ	α
4	2.03735	4.99296	0.00444	0.33869
4.3	1.91458	4.71894	0.0033	0.30574
4.6	1.80695	4.41445	0.00221	0.26637
4.9	1.67018	4.16159	0.0014	0.24965
5.2	1.54239	3.94162	8.64E-04	0.24671
5.5	1.42646	3.74991	5.39E-04	0.2536
5.8	1.37452	3.57872	3.54E-04	0.25562
6.1	1.38309	3.41981	2.51E-04	0.24688
6.4	1.47786	3.27142	1.99E-04	0.21732
6.7	1.54497	3.1369	1.59E-04	0.18685
7	1.61116	3.01366	1.30E-04	0.15593

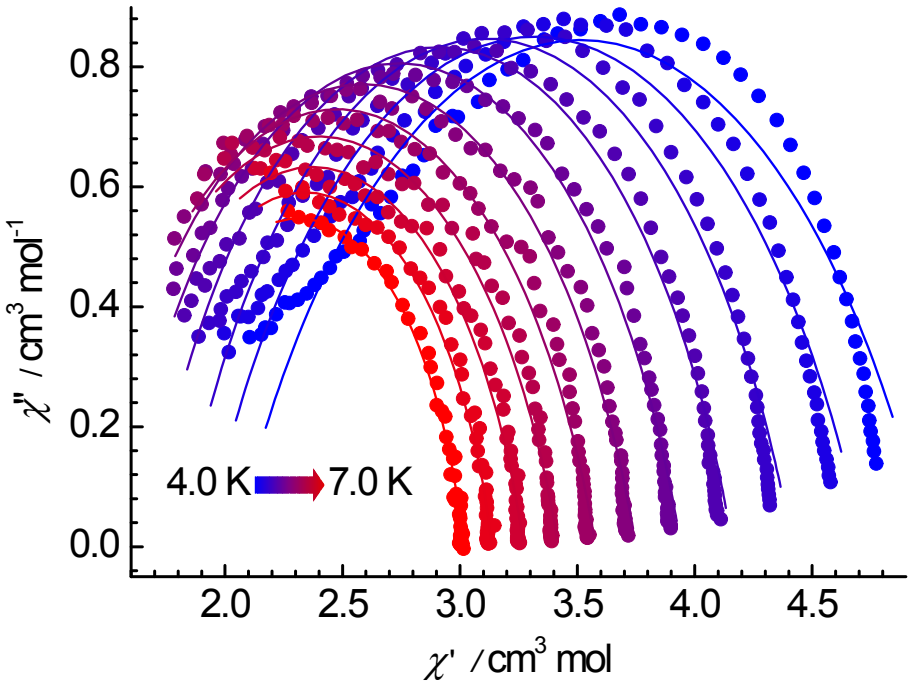

Fig S10 Cole-Cole plots using the frequency-dependence ac susceptibility data under a dc field of 1000 Oe for **3**. The solid lines are the best fits.

4.4 Magnetic data for complex 4

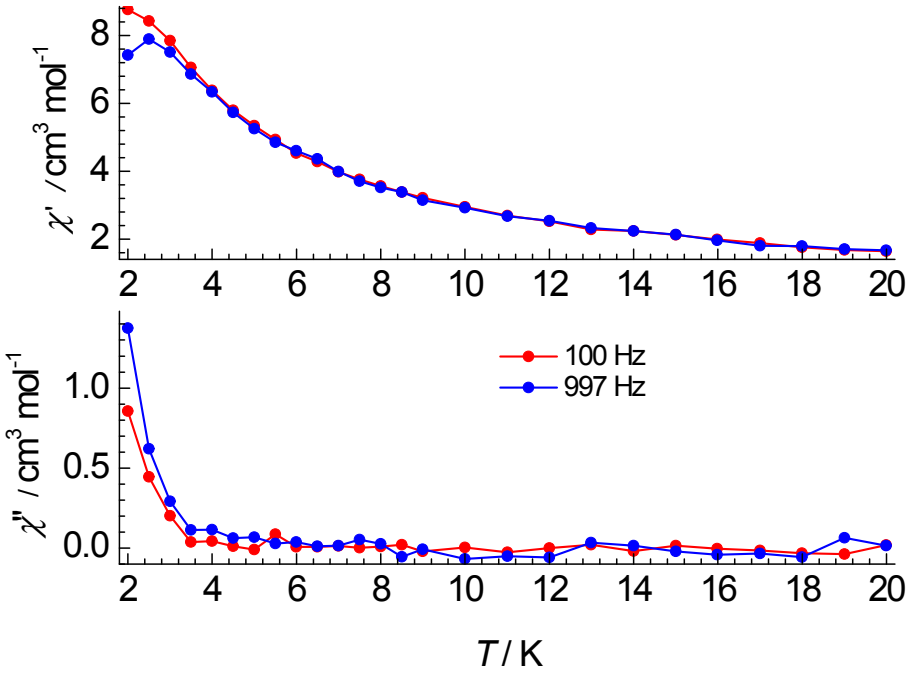

Fig S11. Temperature-dependence of the in-phase (χ', top) and out-of-phase (χ'', bottom) ac susceptibility signals under a dc field of 1000 Oe at the indicated frequencies for **2**, only a small tail is observed.

4.5 Magnetic data for complex 5

Table S16: Relaxation Fitting Parameters of a generalized Debye model for **5**

T	χ_S	χ_T	τ	α
2	0.4712	8.65088	0.61605	0.37439
2.5	0.36087	6.0614	0.21713	0.36487
3	0.31328	4.72856	0.08561	0.30405
3.5	0.2897	3.69144	0.0273	0.18747
4	0.2534	3.11911	0.0096	0.1098
4.5	0.21895	2.7605	0.00377	0.06946
5	0.19324	2.49045	1.64E-03	0.04777
5.5	0.17313	2.27327	7.48E-04	0.03939
6	0.1636	2.09254	3.46E-04	0.03728
6.5	0.14992	1.93501	1.54E-04	0.03871
7	0.11787	1.80163	6.55E-05	0.04548

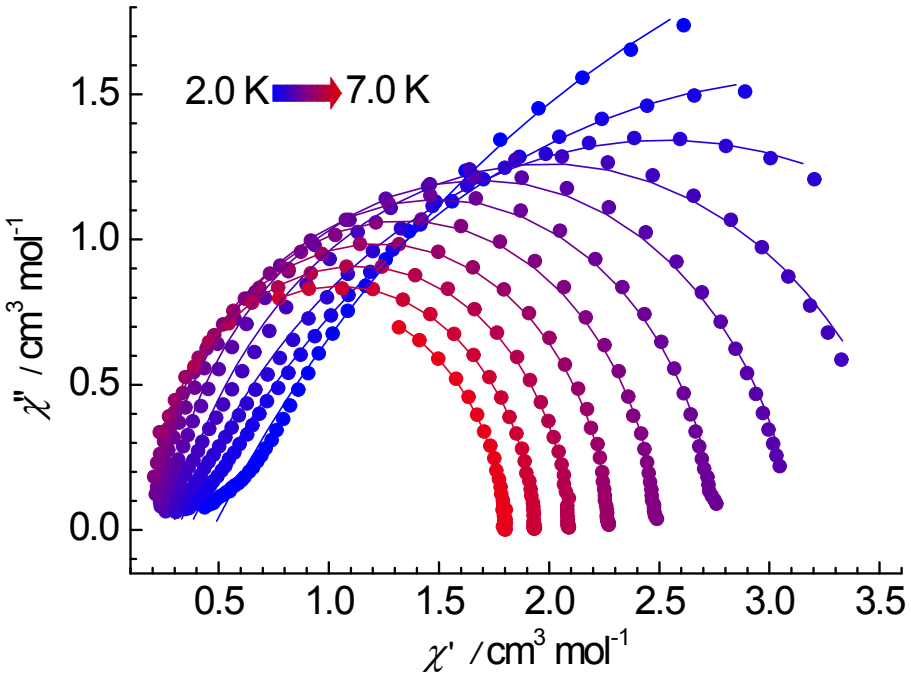

Fig S12 Cole-Cole plots using the frequency-dependence ac susceptibility data under a dc field of 1000 Oe for **5**. The solid lines are the best fits.

4.6 Magnetic data for complex 6

Table S17: Relaxation Fitting Parameters of a generalized Debye model for **6**

T	χ_S	χ_T	τ	α
3	0.42554	4.92967	0.23791	0.29263
3.5	0.38691	3.73343	0.07047	0.18779
4	0.34885	3.12851	0.02574	0.12959
4.5	0.30824	2.75902	0.01097	0.10391
5	0.27605	2.47944	0.00526	0.08821
5.5	0.25395	2.25915	0.00279	0.07885
6	0.23823	2.07803	0.0016	0.07476
6.5	0.22477	1.92263	9.77E-04	0.06813
7	0.21845	1.79219	6.37E-04	0.06789
7.5	0.19971	1.67872	4.28E-04	0.07055
8	0.2128	1.57704	3.08E-04	0.0607
8.5	0.1952	1.48664	2.18E-04	0.06434
9	0.18846	1.40598	1.62E-04	0.05836
9.5	0.17866	1.33539	1.22E-04	0.05965
10	0.17715	1.27146	9.60E-05	0.04889

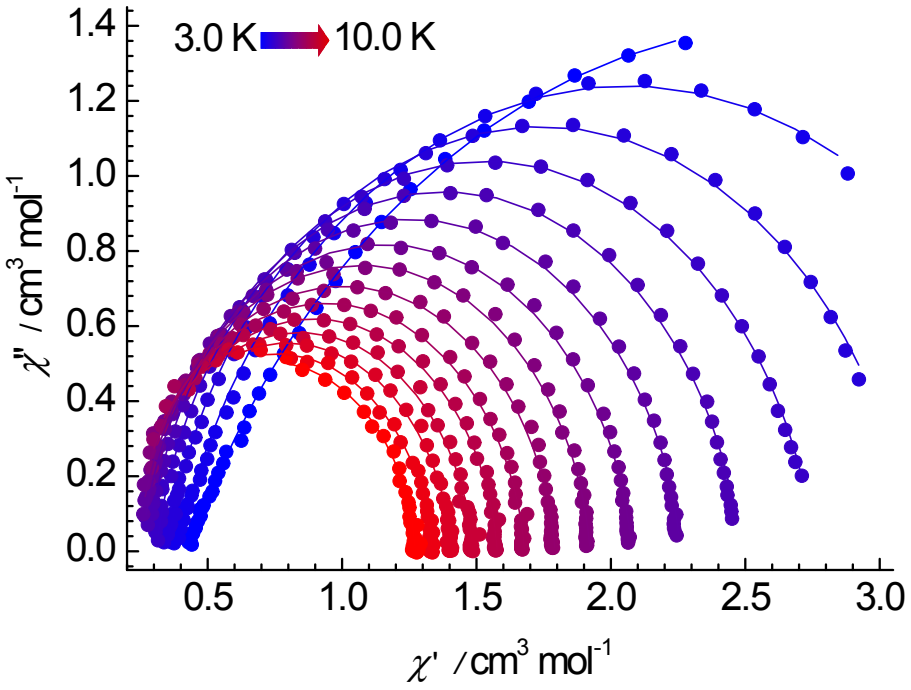

Fig S13 Cole-Cole plots using the frequency-dependence ac susceptibility data under a dc field of 1000 Oe for **6**. The solid lines are the best fits.

5. Potential relaxation processes analysis

To have a further analysis of the relaxation times, other potential relaxation processes are taken into account, including direct, Raman, and Orbach relaxation processes et al. Equations (1)-(4) are used to simulate the relaxation times for complexes **1**, **5** and **6**. For complex **3**, the Orbach relaxation process is obviously dominant, so that further analysis is unnecessary.

$\tau^{-1} = CT^{n}$ Equation (1)

$\tau^{-1} = \tau_{QTM}^{-1} + \tau_{0}^{-1}\exp(-\Delta E/T)$ Equation (2)

$\tau^{-1} = \tau_{QTM}^{-1} + CT^{n}$ Equation (3)

$\tau^{-1} = \tau_{QTM}^{-1} + \tau_{0}^{-1}\exp(-\Delta E/T) + CT^{n}$ Equation (4)

The τ_{QTM} represents temperature-independent QTM. The CT^{n} represents a two-phonon Raman process. Parameters obtained are list below and discussed as details.

5.1 The relaxation times for complex 1

As shown in Figure S16, fitting the relaxation times for complex **1** with equations (1)-(3) couldn't give an ideal result. And for equation (4), over parameterizations also lead to a bad result. Those results could probably owe to a wide contribution of the relaxation times for complex **1**.

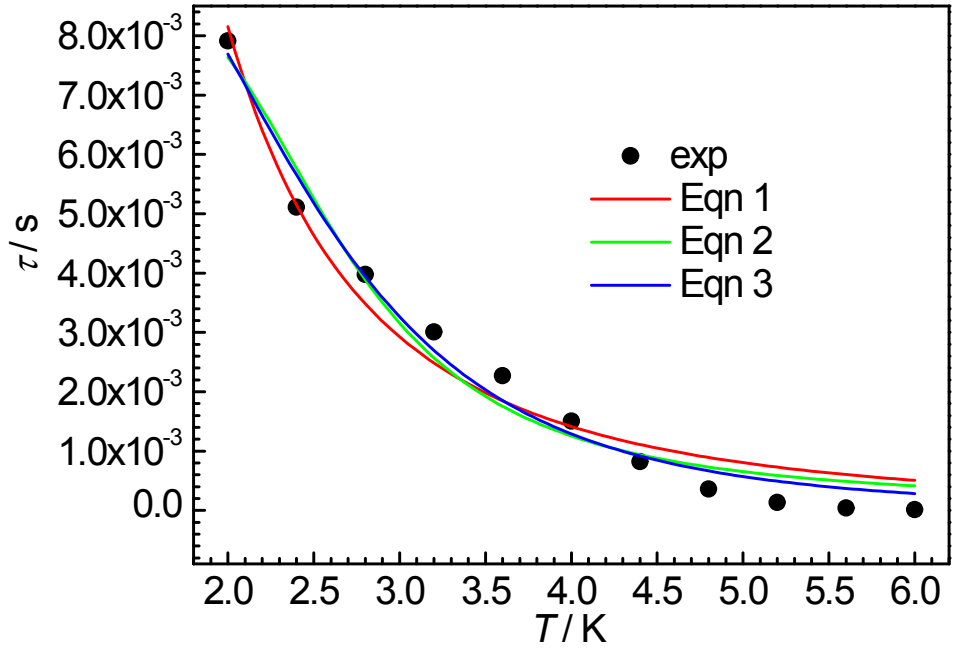

Fig S16 Plots of ln(τ) versus 1/T for **1**, The solid lines are best fits.

5.2 The relaxation times for complex 5

For complex **5**, all of the four equations were used to fit the relaxation times, giving $C = 0.053\ s^{-1}\ K^n$ with n = 4.92 for equation (1); $\tau_{QTM} = 0.88$ s,$\tau_0 = 1.25 \times 10^{-4}$ s and $\Delta E = 19.4$ K for equation (2); $\tau_{QTM} = 1.57$ s, $C = 0.014\ s^{-1}\ K^n$ with n = 6.19 for equation (3); $\tau_{QTM} = 1.01 \times 10^{12}$ s, $C = 0.066\ s^{-1}\ K^n$ with n = 4.62, $\tau_0 = 6.86 \times 10^{-8}$ s and $\Delta E = 48.7$ K for equation (4). Here we can guess that at low temperature, the Raman process may be dominant. The large curvature at low temperature is probably caused by QTM.

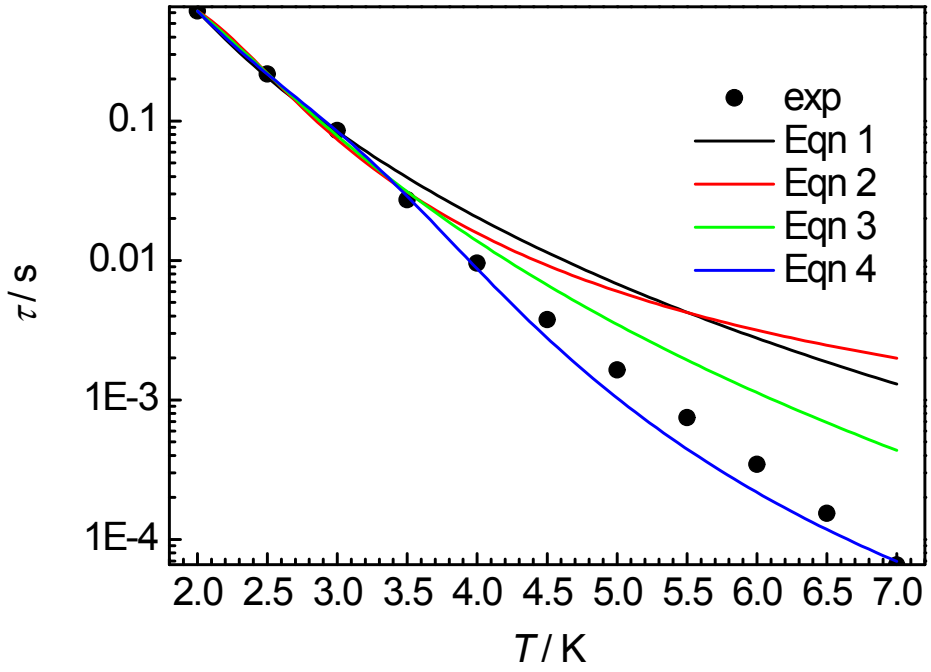

Fig S17 Plots of ln(τ) versus 1/T for **5**, The solid lines are best fits.

5.3 The relaxation times for complex 6

For complex **6**, equations (1)-(3) were used to fit the relaxation times, giving C = 8.00× 10^{-4} s^{-1} K^n with n = 7.80 for equation (1); τ_{QTM} = 0.83 s,τ_0 = 1.21× 10^{-5} s and ΔE = 30.7 K for equation (2); τ_{QTM} = 4.00 × 10^{16} s, C = 8.00 × 10^{-4} s^{-1} K^n with n = 7.80 for equation (3). Here we can also guess that at low temperature, the Raman process may be dominant.

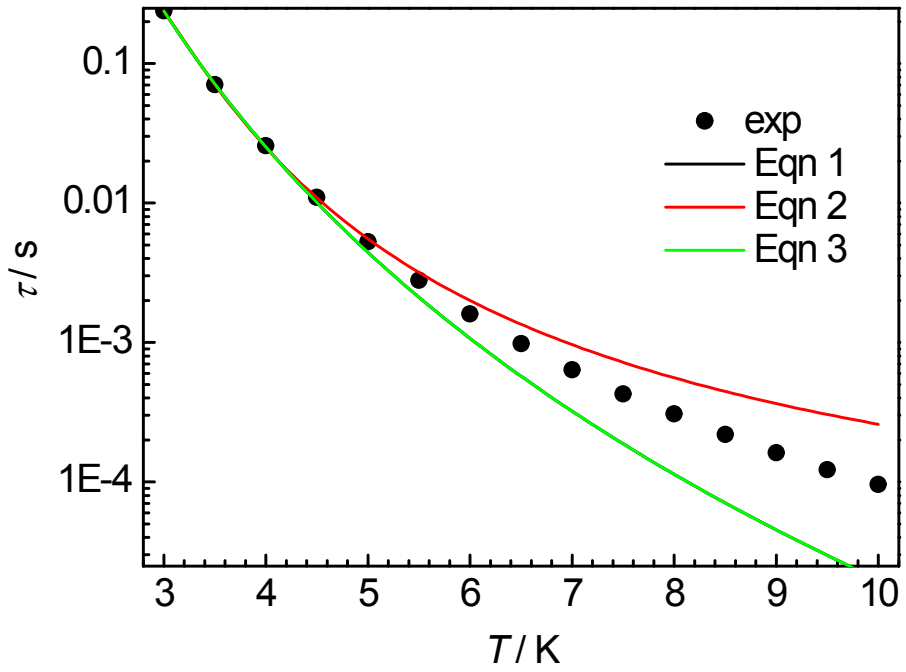

Fig S18 Plots of ln(τ) versus 1/T for **6**, The solid lines are best fits.