

Electronic Supplementary Information

Modulating single-molecule magnet behaviour of phenoxo-O bridged lanthanide(III) dinuclear complexes by using different β -diketonate coligands

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Tables S1. Selected bond lengths (Å) and angles (°) for complex **1**^a

Dy(1)-O(3)	2.304(3)	Dy(1)-O(5)	2.327(3)
Dy(1)-O(1)#1	2.322(3)	Dy(1)-O(2)	2.357(3)
Dy(1)-O(4)	2.327(3)	Dy(1)-O(1)	2.377(3)
Dy(1)-N(1)	2.455(3)	Dy(1)-N(2)	2.665(3)
O(3)-Dy(1)-O(1)#1	87.92(11)	O(4)-Dy(1)-O(2)	150.11(11)
O(3)-Dy(1)-O(4)	78.40(11)	O(5)-Dy(1)-O(2)	138.12(11)
O(1)#1-Dy(1)-O(4)	81.68(10)	O(3)-Dy(1)-O(1)	139.15(10)
O(3)-Dy(1)-O(5)	147.18(11)	O(1)#1-Dy(1)-O(1)	71.28(10)
O(1)#1-Dy(1)-O(5)	98.93(10)	O(4)-Dy(1)-O(1)	129.86(9)
O(4)-Dy(1)-O(5)	71.01(10)	O(5)-Dy(1)-O(1)	72.52(10)
O(3)-Dy(1)-O(2)	71.72(12)	O(2)-Dy(1)-O(1)	76.10(10)
O(1)#1-Dy(1)-O(2)	96.49(10)		

^aSymmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+3/2,-z+1**Tables S2.** Selected bond lengths (Å) and angles (°) for complex **2**^a

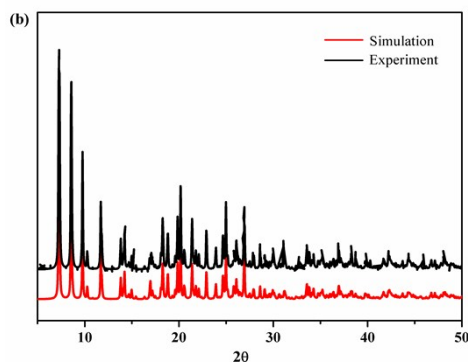
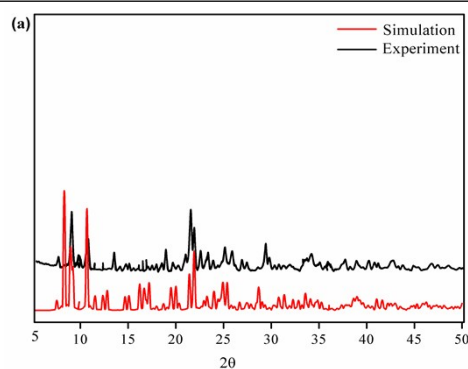
Dy(1)-O(1)#1	2.311(4)	Dy(1)-O(4)	2.335(5)
Dy(1)-O(3)	2.319(5)	Dy(1)-O(5)	2.350(5)
Dy(1)-O(2)	2.333(5)	Dy(1)-O(1)	2.414(4)
Dy(1)-N(1)	2.470(6)	Dy(1)-N(2)	2.658(6)
O(1)#1-Dy(1)-O(3)	88.38(17)	O(2)-Dy(1)-O(5)	150.10(17)
O(1)#1-Dy(1)-O(2)	104.31(17)	O(4)-Dy(1)-O(5)	70.06(17)
O(3)-Dy(1)-O(2)	72.35(18)	O(1)#1-Dy(1)-O(1)	71.33(19)
O(1)#1-Dy(1)-O(4)	89.80(17)	O(3)-Dy(1)-O(1)	136.61(16)
O(3)-Dy(1)-O(4)	148.79(18)	O(2)-Dy(1)-O(1)	76.11(16)
O(2)-Dy(1)-O(4)	137.85(18)	O(4)-Dy(1)-O(1)	71.20(16)
O(1)#1-Dy(1)-O(5)	82.31(17)	O(5)-Dy(1)-O(1)	132.63(16)
O(3)-Dy(1)-O(5)	78.82(18)		

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

Tables S3. Selected bond lengths (Å) and angles (°) for complex **3^a**

Dy(1)-O(4)	2.293(3)	Dy(1)-O(5)	2.343(3)
Dy(1)-O(2)	2.312(3)	Dy(1)-O(1)#1	2.357(3)
Dy(1)-O(3)	2.319(3)	Dy(1)-O(1)	2.386(3)
Dy(1)-N(1)	2.485(4)	Dy(1)-N(2)	2.694(4)
Dy(2)-O(10)	2.286(3)	Dy(2)-O(6)#2	2.309(3)
Dy(2)-O(8)	2.312(3)	Dy(2)-O(7)	2.332(3)
Dy(2)-O(9)	2.340(3)	Dy(2)-O(6)	2.427(3)
Dy(2)-N(3)	2.483(4)	Dy(2)-N(4)	2.663(4)
O(4)-Dy(1)-O(2)	146.89(12)	O(4)-Dy(1)-O(3)	77.46(12)
O(2)-Dy(1)-O(3)	71.80(11)	O(4)-Dy(1)-O(5)	70.99(11)
O(2)-Dy(1)-O(5)	140.94(12)	O(3)-Dy(1)-O(5)	133.36(11)
O(4)-Dy(1)-O(1)#1	80.51(11)	O(2)-Dy(1)-O(1)#1	87.55(11)
O(3)-Dy(1)-O(1)#1	90.29(11)	O(5)-Dy(1)-O(1)#1	116.51(11)
O(4)-Dy(1)-O(1)	123.83(12)	O(2)-Dy(1)-O(1)	79.41(11)
O(3)-Dy(1)-O(1)	145.79(11)	O(5)-Dy(1)-O(1)	80.84(11)
O(1)#1-Dy(1)-O(1)	70.06(12)	O(10)-Dy(2)-O(6)#2	95.88(12)
O(10)-Dy(2)-O(8)	146.03(12)	O(6)#2-Dy(2)-O(8)	85.57(11)
O(10)-Dy(2)-O(7)	142.19(12)	O(6)#2-Dy(2)-O(7)	94.83(12)
O(8)-Dy(2)-O(7)	70.93(11)	O(10)-Dy(2)-O(9)	71.65(12)
O(6)#2-Dy(2)-O(9)	88.17(12)	O(8)-Dy(2)-O(9)	74.48(11)
O(7)-Dy(2)-O(9)	144.91(11)	O(10)-Dy(2)-O(6)	76.58(12)
O(6)#2-Dy(2)-O(6)	70.76(13)	O(8)-Dy(2)-O(6)	134.52(11)
O(7)-Dy(2)-O(6)	73.02(11)	O(9)-Dy(2)-O(6)	139.60(11)

^aSymmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1; #2 -x+2,-y+2,-z



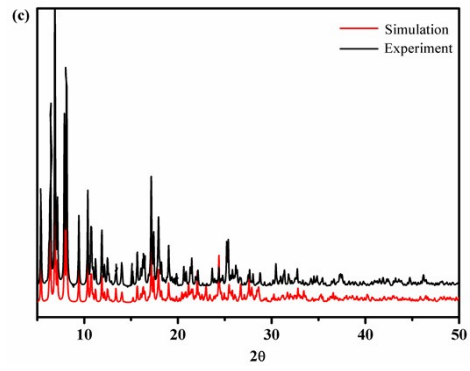


Fig. S1. PXR D patterns for 1(a), 2(b) and 3(c).

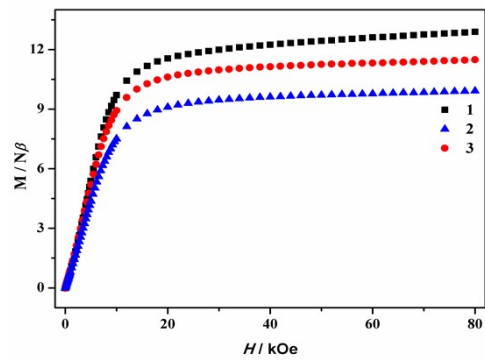


Fig. S2 M versus H plots for 1-3 at 2 K.