Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Modulation of magnetic relaxation behaviors *via* replacing coordinated solvents in a series of linear tetranuclear Dy_4 complexes

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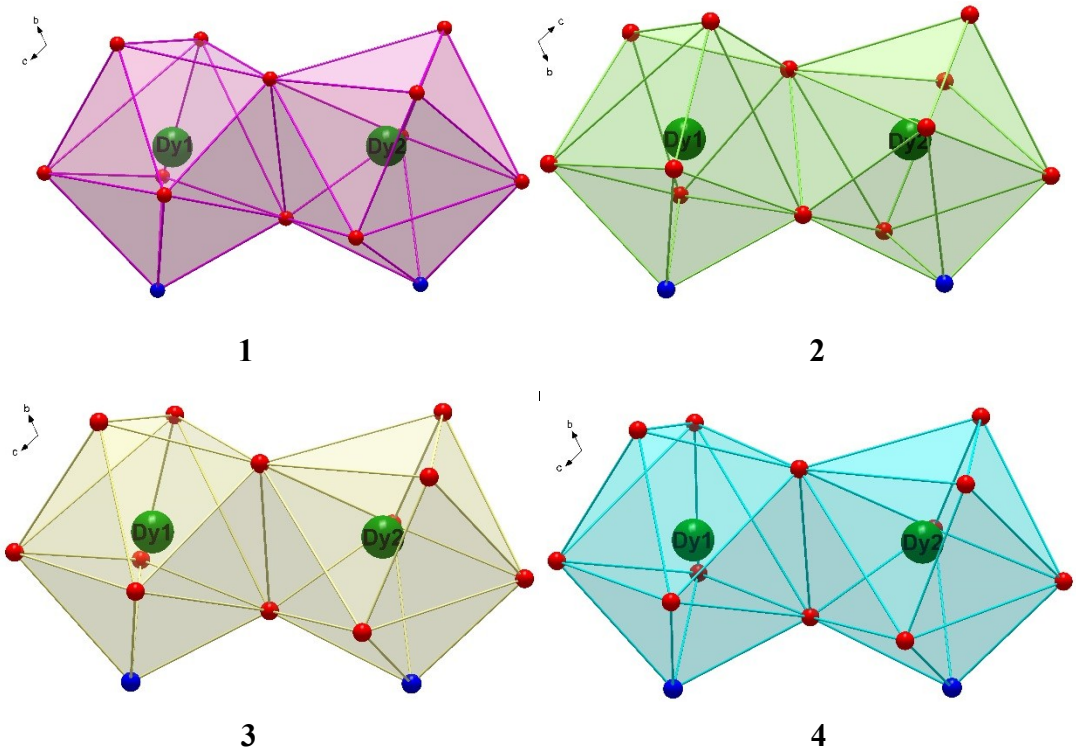


Fig. S1 Coordination polyhedra of Dy(III) ions of **1**-**4** viewed along the *a* axis.

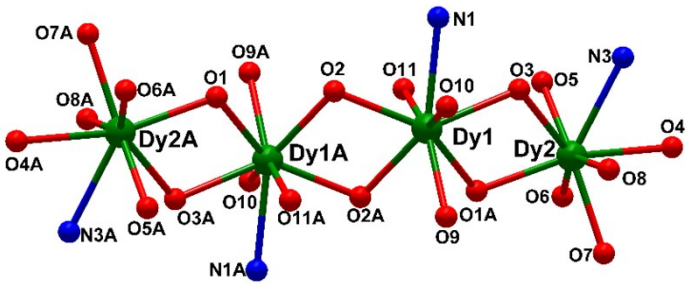
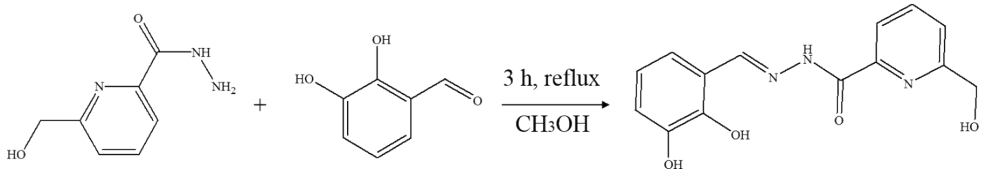


Fig. S2 The structure of linear Dy_4 core in compound **1**.



Scheme S1 The systhesis route for H_3L.

Table S1 Selected bond lengths (Å) and angles (°) for compound 1

Dy(1)-O(1)#1	2.384(5)	Dy(2)-O(1)#1	2.303(5)
Dy(1)-O(5)	2.305(5)	Dy(2)-O(9)	2.368(5)
Dy(1)-O(3)	2.313(5)	Dy(2)-O(7)	2.314(5)
Dy(1)-O(6)	2.306(5)	Dy(2)-O(3)	2.327(5)
Dy(1)-O(2)#1	2.344(5)	Dy(2)-O(8)	2.333(5)
Dy(1)-O(2)	2.258(5)	Dy(2)-O(4)	2.394(5)
Dy(1)-O(11)	2.488(5)	Dy(2)-O(10)	2.294(5)
Dy(1)-N(1)	2.502(6)	Dy(2)-N(3)	2.538(6)
O(1)#1-Dy(1)-O(11)	73.26(18)	O(1)#1-Dy(2)-O(9)	94.60(17)
O(1)#1-Dy(1)-N(1)	127.79(17)	O(1)#1-Dy(2)-O(7)	87.34(18)
O(5)-Dy(1)-O(1)#1	131.58(19)	O(1)#1-Dy(2)-O(3)	70.00(17)
O(5)-Dy(1)-O(3)	89.55(19)	O(1)#1-Dy(2)-O(8)	98.10(18)
O(5)-Dy(1)-O(11)	147.06(19)	O(1)#1-Dy(2)-O(4)	162.62(19)
O(5)-Dy(1)-O(6)	70.89(19)	O(1)#1-Dy(2)-N(3)	133.58(19)
O(5)-Dy(1)-O(2)#1	130.13(18)	O(9)-Dy(2)-O(4)	89.60(19)
O(5)-Dy(1)-N(1)	70.22(19)	O(9)-Dy(2)-N(3)	67.89(19)
O(3)-Dy(1)-O(1)#1	68.83(17)	O(7)-Dy(2)-O(9)	145.23(19)
O(3)-Dy(1)-O(11)	80.04(19)	O(7)-Dy(2)-O(3)	135.02(18)
O(3)-Dy(1)-O(2)#1	135.64(17)	O(7)-Dy(2)-O(8)	71.11(18)
O(3)-Dy(1)-N(1)	64.35(19)	O(7)-Dy(2)-O(4)	79.72(19)
O(11)-Dy(1)-N(1)	77.13(19)	O(7)-Dy(2)-N(3)	131.76(19)
O(6)-Dy(1)-O(1)#1	74.43(17)	O(3)-Dy(2)-O(9)	77.02(18)
O(6)-Dy(1)-O(3)	106.14(19)	O(3)-Dy(2)-O(8)	74.26(17)
O(6)-Dy(1)-O(11)	142.0(2)	O(3)-Dy(2)-O(4)	127.36(18)
O(6)-Dy(1)-O(2)#1	75.85(18)	O(3)-Dy(2)-N(3)	64.35(18)
O(6)-Dy(1)-N(1)	139.91(19)	O(8)-Dy(2)-O(9)	142.20(19)
O(2)#1-Dy(1)-O(1)#1	69.33(16)	O(8)-Dy(2)-O(4)	88.7(2)
O(2)-Dy(1)-O(1)#1	138.15(17)	O(8)-Dy(2)-N(3)	77.70(19)
O(2)-Dy(1)-O(5)	87.49(19)	O(4)-Dy(2)-N(3)	63.4(2)
O(2)-Dy(1)-O(3)	135.94(17)	O(10)-Dy(2)-O(1)#1	85.63(19)
O(2)#1-Dy(1)-O(11)	74.47(19)	O(10)-Dy(2)-O(9)	70.4(2)
O(2)-Dy(1)-O(11)	79.04(19)	O(10)-Dy(2)-O(7)	75.2(2)
O(2)-Dy(1)-O(6)	114.20(18)	O(10)-Dy(2)-O(3)	137.3(2)
O(2)-Dy(1)-O(2)#1	73.4(2)	O(10)-Dy(2)-O(8)	145.8(2)
O(2)-Dy(1)-N(1)	73.38(18)	O(10)-Dy(2)-O(4)	79.9(2)
O(2)#1-Dy(1)-N(1)	139.57(18)	O(10)-Dy(2)-N(3)	123.32(19)

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

Table S2 Selected bond lengths (Å) and angles (°) for compound 2

Dy(1)-O(2)#1	2.355(4)	Dy(2)-O(10)	2.314(5)
Dy(1)-O(2)	2.272(4)	Dy(2)-O(3)	2.340(4)
Dy(1)-O(5)	2.303(4)	Dy(2)-O(8)	2.388(4)
Dy(1)-O(3)	2.305(4)	Dy(2)-O(1)#1	2.320(4)
Dy(1)-O(6)	2.316(4)	Dy(2)-O(7)	2.319(4)

Dy(1)-O(11)	2.477(5)	Dy(2)-O(9)	2.343(4)
Dy(1)-O(1)#1	2.373(4)	Dy(2)-O(4)	2.391(5)
Dy(1)-N(1)	2.508(5)	Dy(2)-N(3)	2.526(5)
O(2)-Dy(1)-O(2)#1	73.68(16)	O(10)-Dy(2)-O(3)	138.56(16)
O(2)-Dy(1)-O(5)	88.38(16)	O(10)-Dy(2)-O(8)	143.68(16)
O(2)-Dy(1)-O(3)	136.62(18)	O(10)-Dy(2)-O(1)#1	85.96(16)
O(2)-Dy(1)-O(6)	111.95(16)	O(10)-Dy(2)-O(7)	73.81(16)
O(2)#1-Dy(1)-O(11)	75.91(15)	O(10)-Dy(2)-O(9)	71.22(16)
O(2)-Dy(1)-O(11)	79.86(16)	O(10)-Dy(2)-O(4)	81.29(18)
O(2)-Dy(1)-O(1)#1	139.39(14)	O(10)-Dy(2)-N(3)	125.08(16)
O(2)#1-Dy(1)-O(1)#1	69.20(14)	O(3)-Dy(2)-O(8)	74.61(14)
O(2)-Dy(1)-N(1)	73.61(18)	O(3)-Dy(2)-O(9)	78.62(15)
O(2)#1-Dy(1)-N(1)	139.68(15)	O(3)-Dy(2)-O(4)	126.91(16)
O(5)-Dy(1)-O(2)#1	131.99(15)	O(3)-Dy(2)-N(3)	64.19(16)
O(5)-Dy(1)-O(3)	87.79(16)	O(8)-Dy(2)-O(4)	86.70(18)
O(5)-Dy(1)-O(6)	70.47(16)	O(8)-Dy(2)-N(3)	77.57(16)
O(5)-Dy(1)-O(11)	145.08(16)	O(1)#1-Dy(2)-O(3)	69.28(14)
O(5)-Dy(1)-O(1)#1	129.09(16)	O(1)#1-Dy(2)-O(8)	97.86(16)
O(5)-Dy(1)-N(1)	69.41(16)	O(1)#1-Dy(2)-O(9)	95.82(16)
O(3)-Dy(1)-O(2)#1	135.20(14)	O(1)#1-Dy(2)-O(4)	163.76(16)
O(3)-Dy(1)-O(6)	107.28(16)	O(1)#1-Dy(2)-N(3)	132.78(16)
O(3)-Dy(1)-O(11)	79.02(16)	O(7)-Dy(2)-O(3)	133.95(15)
O(3)-Dy(1)-O(1)#1	68.96(14)	O(7)-Dy(2)-O(8)	70.40(15)
O(3)-Dy(1)-N(1)	64.68(15)	O(7)-Dy(2)-O(1)#1	86.74(15)
O(6)-Dy(1)-O(2)#1	75.71(15)	O(7)-Dy(2)-O(9)	144.64(16)
O(6)-Dy(1)-O(11)	144.34(16)	O(7)-Dy(2)-O(4)	80.10(16)
O(6)-Dy(1)-O(1)#1	74.29(15)	O(7)-Dy(2)-N(3)	132.31(16)
O(6)-Dy(1)-N(1)	139.26(16)	O(9)-Dy(2)-O(8)	143.15(16)
O(11)-Dy(1)-N(1)	75.73(16)	O(9)-Dy(2)-O(4)	89.57(17)
O(1)#1-Dy(1)-O(11)	75.74(15)	O(9)-Dy(2)-N(3)	68.10(16)
O(1)#1-Dy(1)-N(1)	128.98(15)	O(4)-Dy(2)-N(3)	63.39(17)

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

Table S3 Selected bond lengths (Å) and angles (°) for compound 3

Dy(1)-O(3)	2.298(6)	Dy(2)-O(3)	2.343(6)
Dy(1)-O(6)	2.305(7)	Dy(2)-O(9)	2.318(7)
Dy(1)-O(5)	2.308(8)	Dy(2)-O(7)	2.309(7)
Dy(1)-O(2)	2.272(6)	Dy(2)-O(10)	2.346(7)
Dy(1)-O(2)#1	2.348(7)	Dy(2)-O(8)	2.397(7)

Dy(1)-N(1)	2.495(8)	Dy(2)-O(4)	2.388(7)
Dy(1)-O(1)#1	2.359(6)	Dy(2)-N(3)	2.531(8)
Dy(1)-O(11)	2.449(8)	Dy(2)-O(1)#1	2.330(6)
O(3)-Dy(1)-O(6)	110.5(3)	O(3)-Dy(2)-O(10)	79.2(3)
O(3)-Dy(1)-O(5)	89.3(3)	O(3)-Dy(2)-O(8)	75.9(2)
O(3)-Dy(1)-O(2)#1	135.3(2)	O(3)-Dy(2)-O(4)	126.5(2)
O(3)-Dy(1)-N(1)	64.8(2)	O(3)-Dy(2)-N(3)	64.3(2)
O(3)-Dy(1)-O(1)#1	68.6(2)	O(9)-Dy(2)-O(3)	139.0(3)
O(3)-Dy(1)-O(11)	81.1(3)	O(9)-Dy(2)-O(10)	71.1(3)
O(6)-Dy(1)-O(5)	70.0(3)	O(9)-Dy(2)-O(8)	142.2(3)
O(6)-Dy(1)-O(2)#1	73.8(3)	O(9)-Dy(2)-O(4)	81.2(3)
O(6)-Dy(1)-N(1)	139.7(3)	O(9)-Dy(2)-N(3)	124.8(3)
O(6)-Dy(1)-O(1)#1	75.9(3)	O(9)-Dy(2)-O(1)#1	87.6(3)
O(6)-Dy(1)-O(11)	146.1(3)	O(7)-Dy(2)-O(3)	134.4(2)
O(5)-Dy(1)-O(2)#1	130.6(3)	O(7)-Dy(2)-O(9)	72.8(3)
O(5)-Dy(1)-N(1)	69.9(3)	O(7)-Dy(2)-O(10)	143.6(3)
O(5)-Dy(1)-O(1)#1	129.2(3)	O(7)-Dy(2)-O(8)	70.1(3)
O(5)-Dy(1)-O(11)	143.6(3)	O(7)-Dy(2)-O(4)	80.6(3)
O(2)-Dy(1)-O(3)	137.2(2)	O(7)-Dy(2)-N(3)	132.9(3)
O(2)-Dy(1)-O(6)	108.2(3)	O(7)-Dy(2)-O(1)#1	86.7(2)
O(2)-Dy(1)-O(5)	87.2(3)	O(10)-Dy(2)-O(8)	144.0(3)
O(2)-Dy(1)-O(2)#1	73.2(3)	O(10)-Dy(2)-O(4)	88.8(3)
O(2)-Dy(1)-N(1)	74.1(2)	O(10)-Dy(2)-N(3)	67.9(3)
O(2)#1-Dy(1)-N(1)	139.7(2)	O(8)-Dy(2)-N(3)	78.0(3)
O(2)#1-Dy(1)-O(1)#1	69.7(2)	O(4)-Dy(2)-O(8)	85.6(3)
O(2)-Dy(1)-O(1)#1	139.8(2)	O(4)-Dy(2)-N(3)	62.9(3)
O(2)#1-Dy(1)-O(11)	75.9(3)	O(1)#1-Dy(2)-O(3)	68.4(2)
O(2)-Dy(1)-O(11)	76.9(3)	O(1)#1-Dy(2)-O(10)	96.9(3)
O(1)#1-Dy(1)-N(1)	129.1(2)	O(1)#1-Dy(2)-O(8)	97.5(3)
O(1)#1-Dy(1)-O(11)	79.5(3)	O(1)#1-Dy(2)-O(4)	165.0(2)
O(11)-Dy(1)-N(1)	74.3(3)	O(1)#1-Dy(2)-N(3)	132.1(2)

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

Table S4 Selected bond lengths (Å) and angles (°) for compound 4

Dy(1)-O(2)	2.259(4)	Dy(2)-O(9)	2.298(4)
Dy(1)-O(2)#1	2.363(4)	Dy(2)-O(1)#1	2.341(4)
Dy(1)-O(1)#1	2.336(3)	Dy(2)-O(10)	2.343(4)
Dy(1)-O(6)	2.330(4)	Dy(2)-O(7)	2.314(4)
Dy(1)-O(11)	2.484(4)	Dy(2)-O(4)	2.376(4)

Dy(1)-N(1)	2.480(5)	Dy(2)-O(8)	2.397(4)
Dy(1)-O(5)	2.314(4)	Dy(2)-N(3)	2.531(5)
Dy(1)-O(3)	2.292(4)	Dy(2)-O(3)	2.329(3)
O(2)-Dy(1)-O(2)#1	72.18(14)	O(9)-Dy(2)-O(1)#1	87.51(13)
O(2)-Dy(1)-O(1)#1	139.71(12)	O(9)-Dy(2)-O(10)	71.36(14)
O(2)-Dy(1)-O(6)	100.56(15)	O(9)-Dy(2)-O(7)	73.40(14)
O(2)#1-Dy(1)-O(11)	76.10(14)	O(9)-Dy(2)-O(4)	81.14(15)
O(2)-Dy(1)-O(11)	73.78(14)	O(9)-Dy(2)-O(8)	142.75(14)
O(2)#1-Dy(1)-N(1)	139.41(14)	O(9)-Dy(2)-N(3)	124.70(14)
O(2)-Dy(1)-N(1)	74.47(14)	O(9)-Dy(2)-O(3)	136.84(14)
O(2)-Dy(1)-O(5)	94.69(14)	O(1)#1-Dy(2)-O(10)	99.20(14)
O(2)-Dy(1)-O(3)	137.53(13)	O(1)#1-Dy(2)-O(4)	164.38(13)
O(1)#1-Dy(1)-O(2)#1	70.22(12)	O(1)#1-Dy(2)-O(8)	97.52(13)
O(1)#1-Dy(1)-O(11)	83.61(14)	O(1)#1-Dy(2)-N(3)	132.22(13)
O(1)#1-Dy(1)-N(1)	130.03(14)	O(10)-Dy(2)-O(4)	87.34(16)
O(6)-Dy(1)-O(2)#1	71.63(14)	O(10)-Dy(2)-O(8)	142.58(14)
O(6)-Dy(1)-O(1)#1	80.92(14)	O(10)-Dy(2)-N(3)	66.28(15)
O(6)-Dy(1)-O(11)	147.33(15)	O(7)-Dy(2)-O(1)#1	85.99(14)
O(6)-Dy(1)-N(1)	137.73(15)	O(7)-Dy(2)-O(10)	144.07(14)
N(1)-Dy(1)-O(11)	72.89(15)	O(7)-Dy(2)-O(4)	80.53(14)
O(5)-Dy(1)-O(2)#1	135.69(14)	O(7)-Dy(2)-O(8)	70.21(13)
O(5)-Dy(1)-O(1)#1	122.49(14)	O(7)-Dy(2)-N(3)	133.17(15)
O(5)-Dy(1)-O(6)	69.58(15)	O(7)-Dy(2)-O(3)	135.62(13)
O(5)-Dy(1)-O(11)	141.96(15)	O(4)-Dy(2)-O(8)	85.35(15)
O(5)-Dy(1)-N(1)	69.09(15)	O(4)-Dy(2)-N(3)	63.39(14)
O(3)-Dy(1)-O(2)#1	135.68(12)	O(8)-Dy(2)-N(3)	77.70(15)
O(3)-Dy(1)-O(1)#1	69.00(12)	O(3)-Dy(2)-O(1)#1	68.29(12)
O(3)-Dy(1)-O(6)	117.40(15)	O(3)-Dy(2)-O(10)	77.73(14)
O(3)-Dy(1)-O(11)	82.86(15)	O(3)-Dy(2)-O(4)	127.21(13)
O(3)-Dy(1)-N(1)	64.85(13)	O(3)-Dy(2)-O(8)	77.81(13)
O(3)-Dy(1)-O(5)	82.28(15)	O(3)-Dy(2)-N(3)	64.22(14)

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

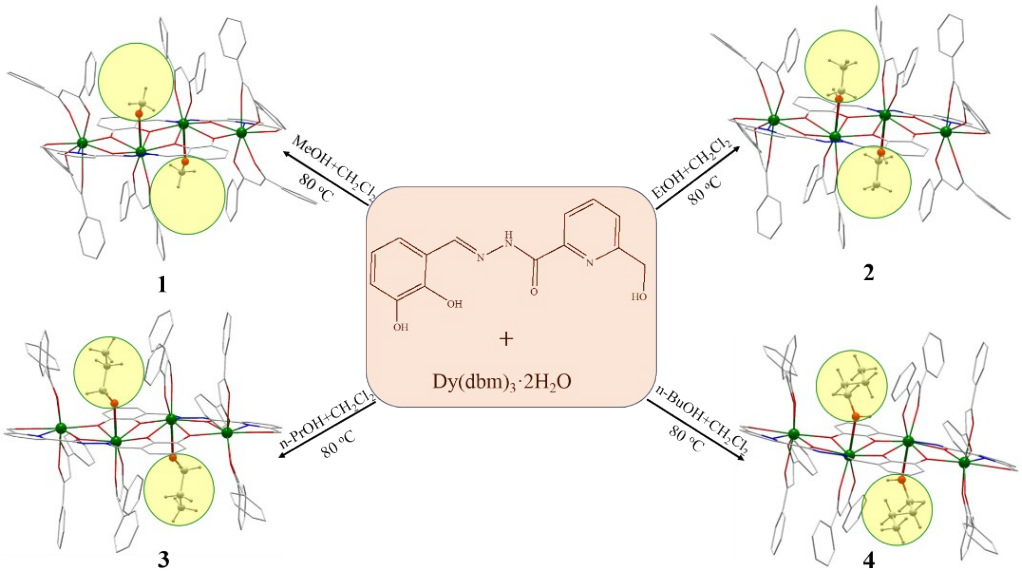


Fig. S3 Molecular structures of **1-4** with different coordinated solvents highlighted by the yellow background circles.

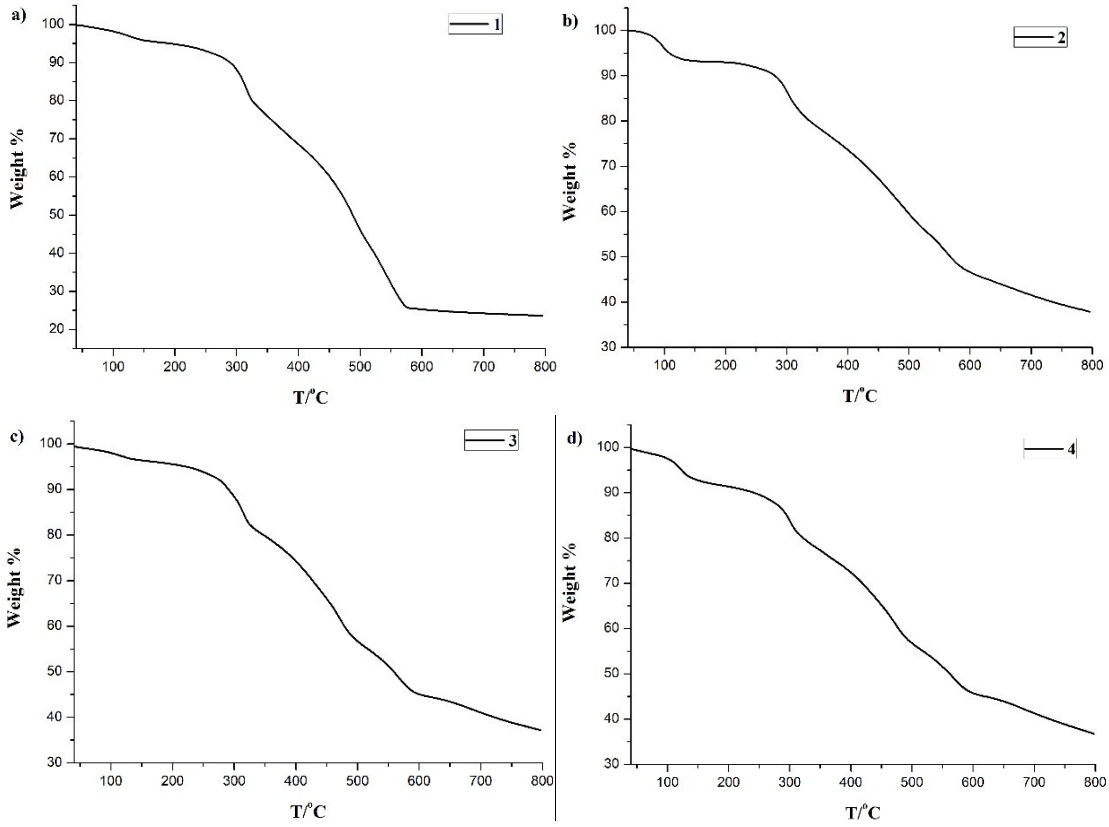


Fig. S4 The TGA curves for compounds **1-4**.

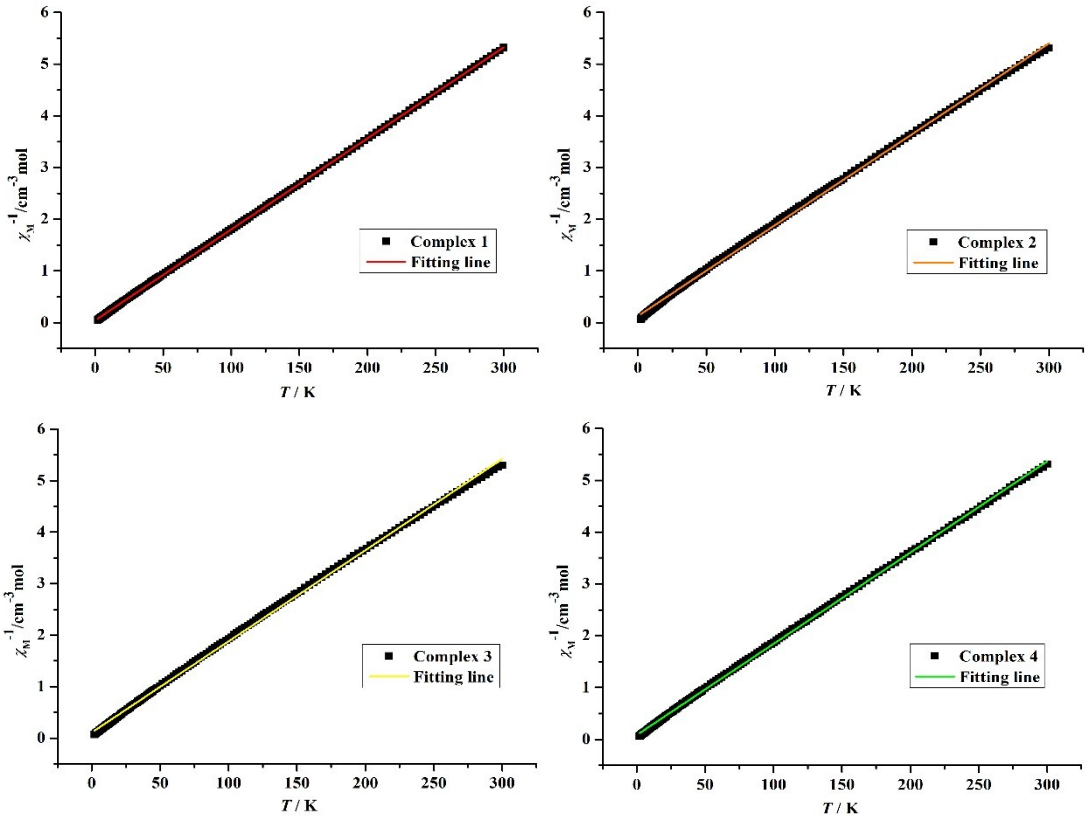


Fig. S5 Plots of χ_M^{-1} *vs. T* for **1**-**4**.

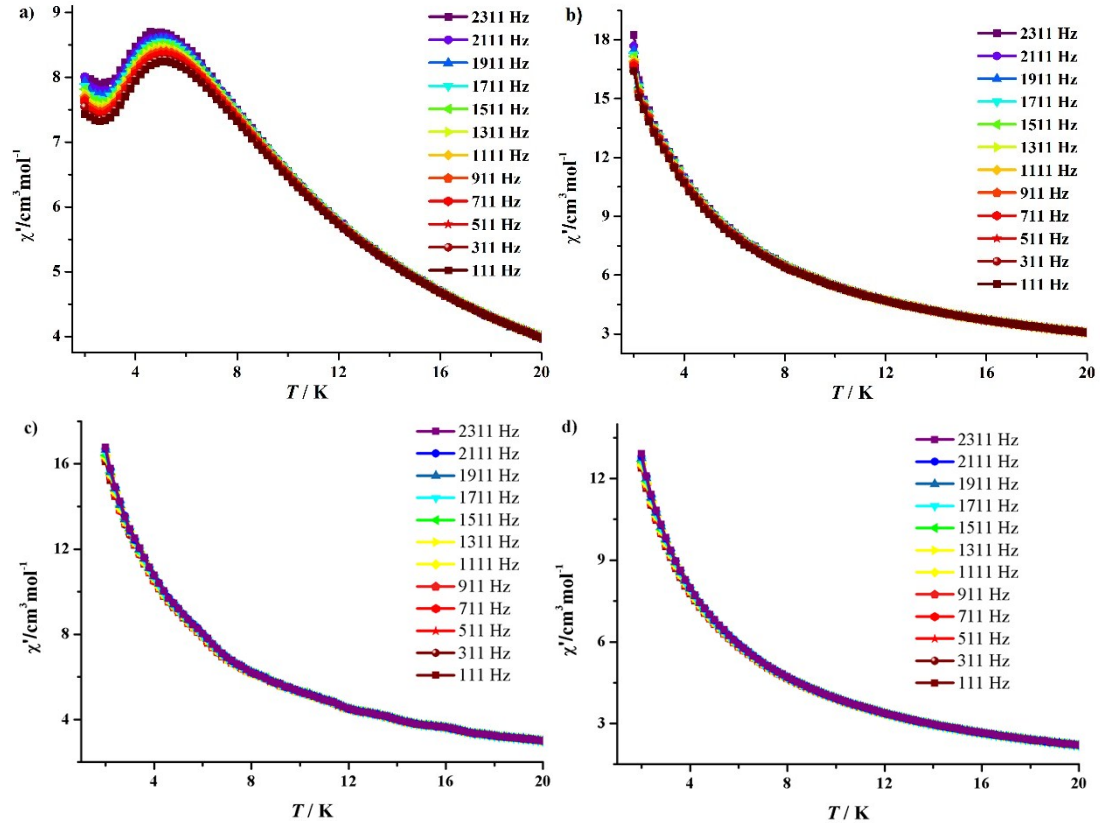


Fig. S6 Temperature dependence of the in-phase (χ′) components of the ac magnetic susceptibility for **1** (a), **2** (b), **3** (c) and **4** (d) under a zero *dc* field.

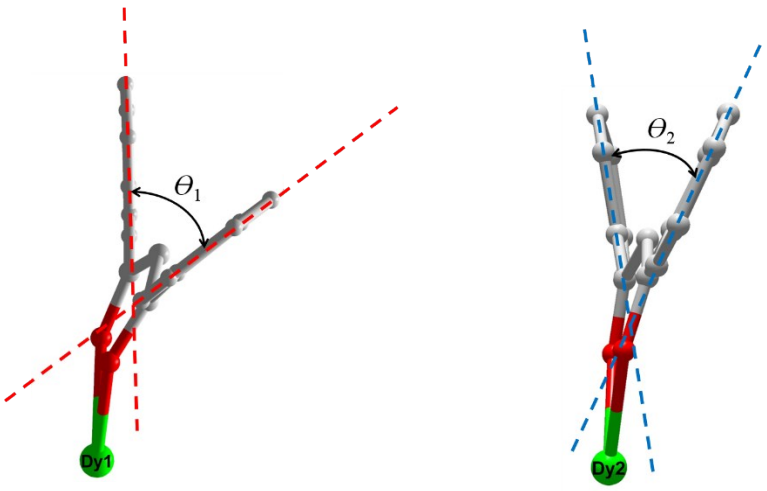


Fig. S7 The torsion angles of ligand dbm coordinated to Dy1 and Dy2 in **1-4**.

Table S5 The comparison of the torsion angles of ligand dbm coordinated to Dy1 and Dy2 in compounds 1-4

Compounds	Θ_1 (°)	Θ_2 (°)
1	16.072	71.931
2	22.137	64.598
3	22.121	55.720
4	35.113	63.403