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

Supporting Information

Single-ion magnets with D_{4d} symmetry based on electron-donating β-diketonate Dy(III) complexes

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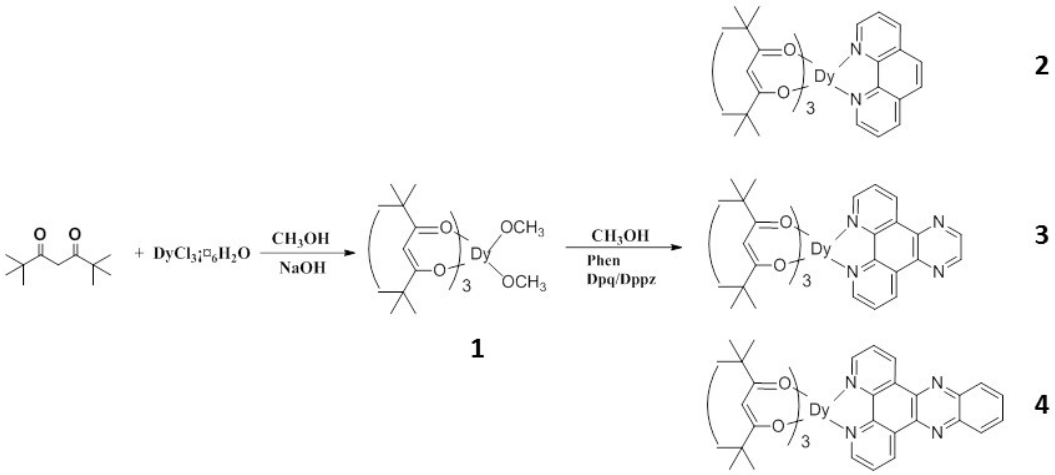
Scheme S1. Synthesis of complexes **1**–**4**.



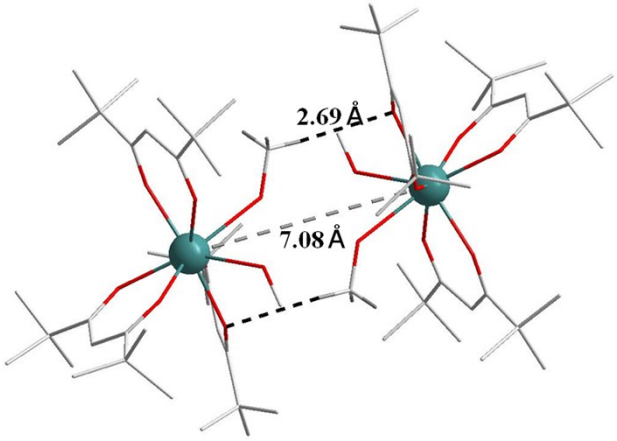


Figure S1. The hydrogen bonds interactions between the molecules in complex **1**.

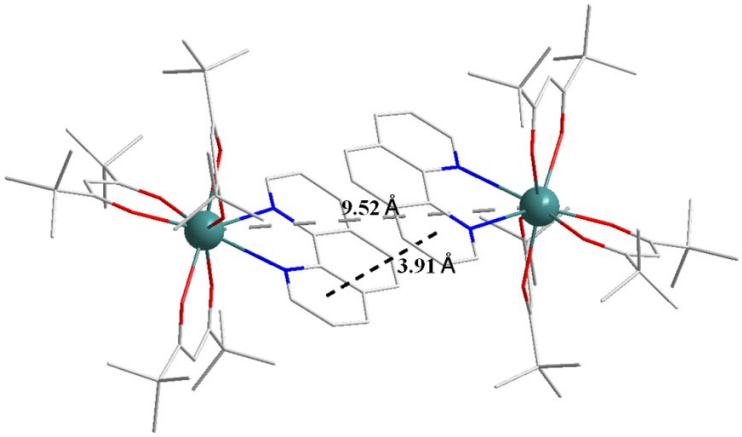


Figure S2. The π-π stacking between the molecules in complex **2**.

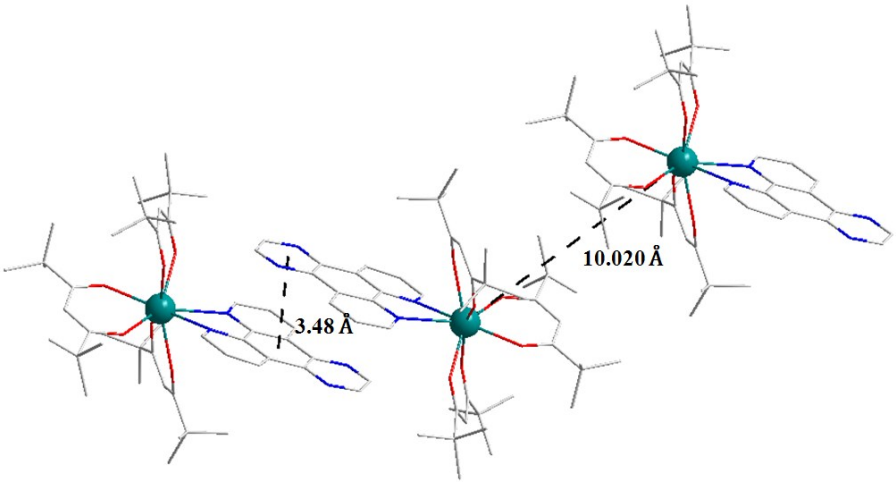


Figure S3. The π-π stacking between the molecules in complex **3**.

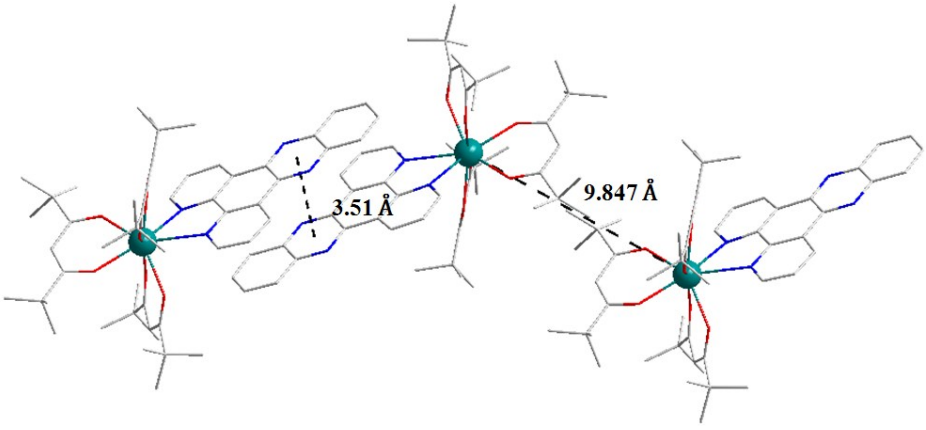


Figure S4. The π-π stacking between the molecules in complex **4**.

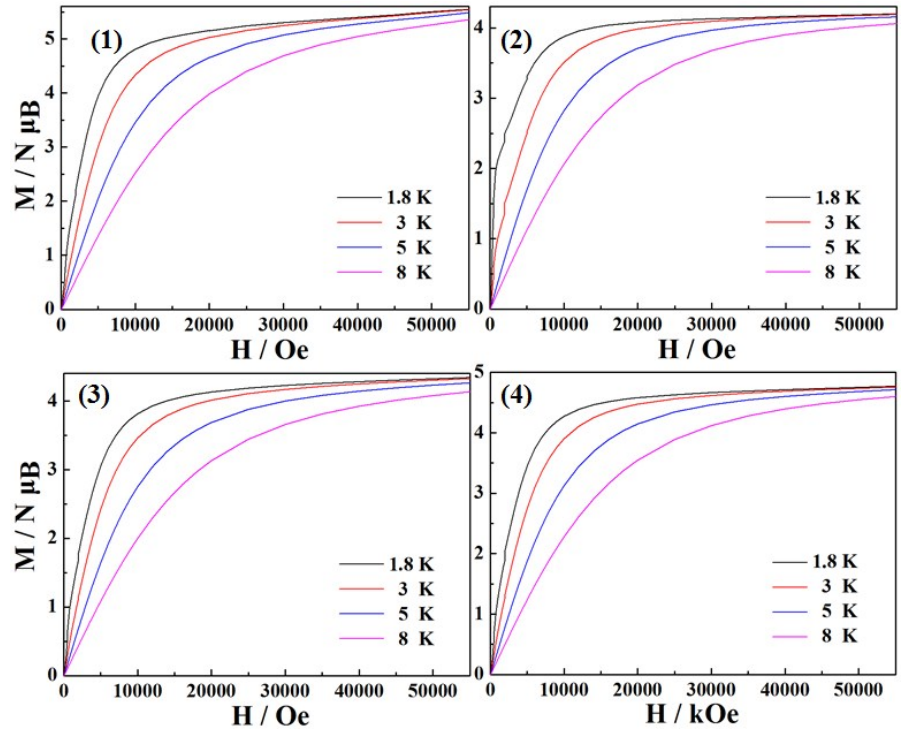


Figure S5. M versus H plots at 1.8 K, 3.0 K, 5.0 K and 8.0 K for complexes **1**−**4**.

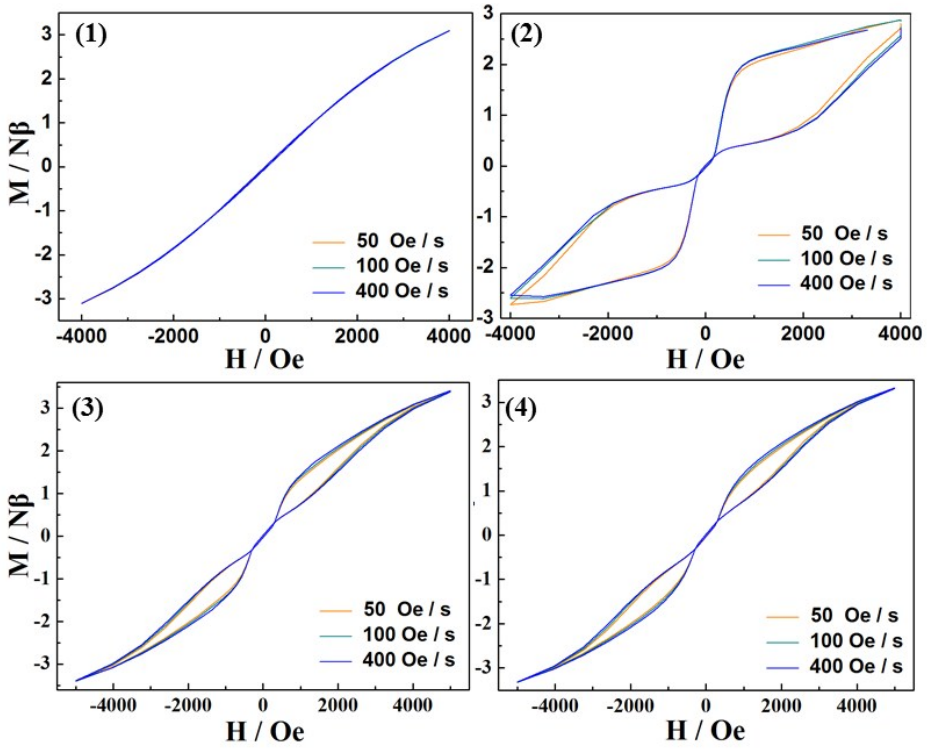


Figure S6. Hysteresis loops for the complexes **1**–**4** at 1.8 K.

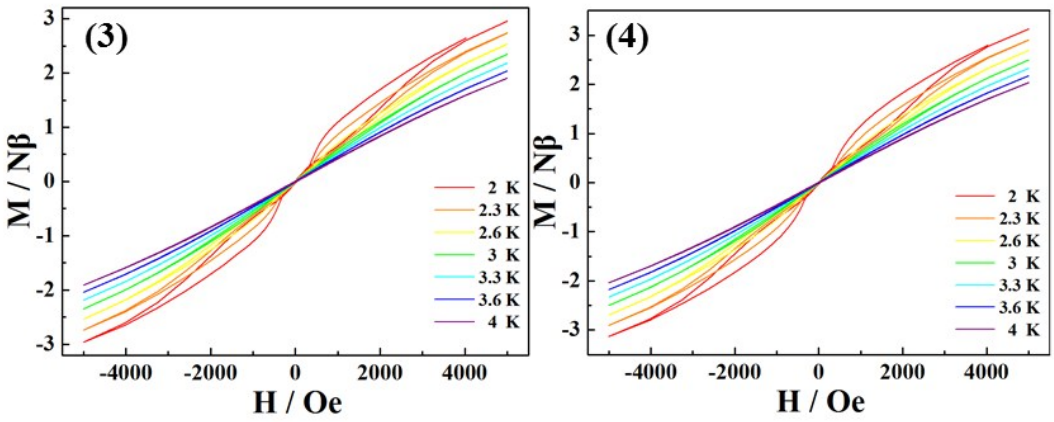


Figure S7. Hysteresis loop for complexes **3** and **4** at various temperatures.

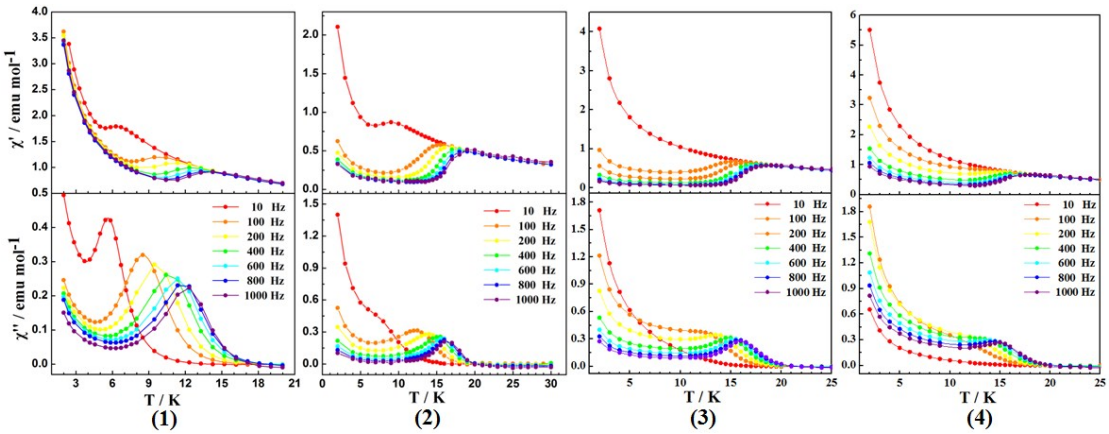


Figure S8. Temperature dependence of the in-phase (χ′) and out-of-phase (χ″) ac susceptibility under 0 Oe in the frequency range 10–1000 Hz for complexes **1**−**4**.

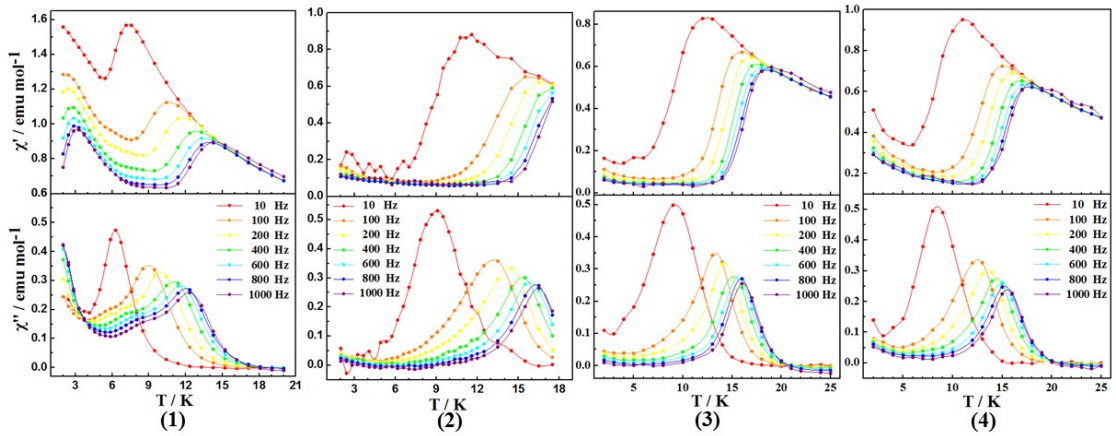


Figure S9. Temperature dependence of the in-phase (χ′) and out-of-phase (χ″) ac susceptibility under 1000 Oe in the frequency range 1–1000 Hz complexes **1**−**4**.

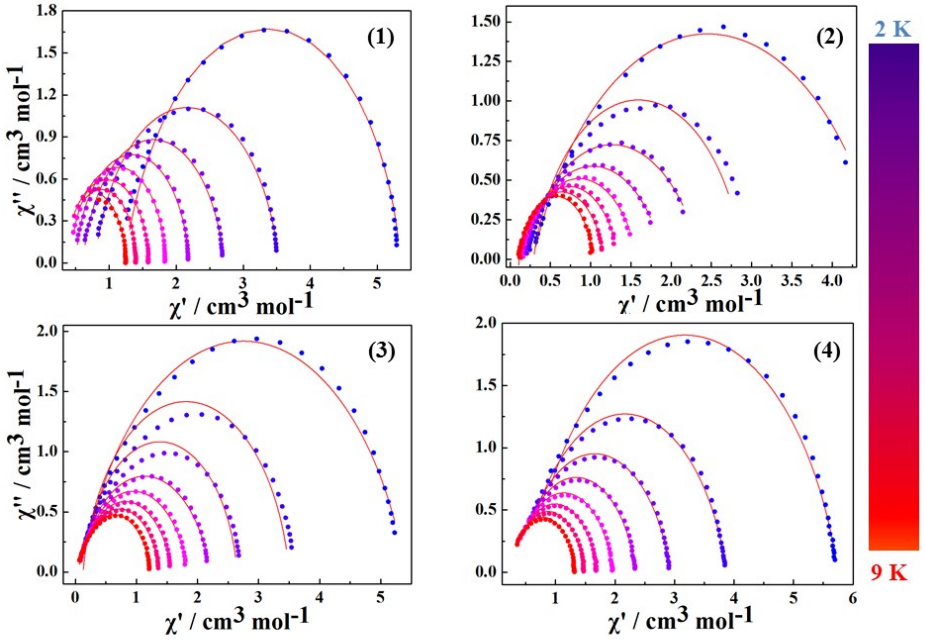


Figure S10. Cole−Cole plots measured at 2−9 K in 0 dc field for complexes **1**−**4**.

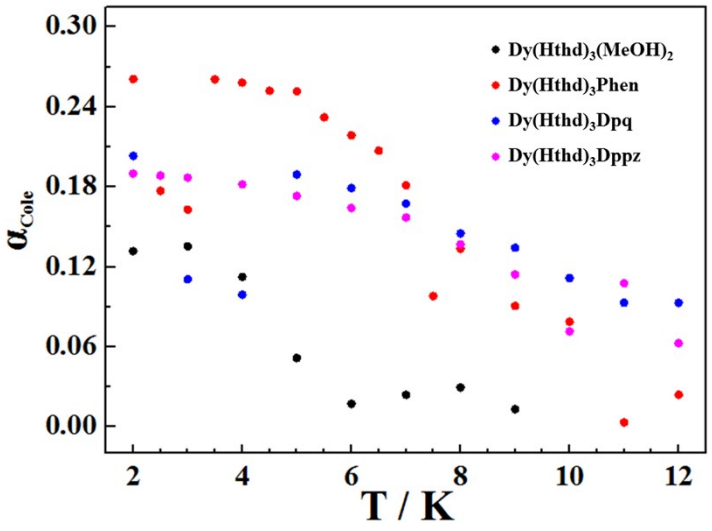


Figure S11. Fitted broadness parameters α_{Cole} as functions of temperature for complexes **1**–**4**.

Table S1. Selected bond lengths (Å) and angles (°) for complexes **1**–**4**.

1		**2**	
Dy(1)–O(1)	2.293(3)	Dy(1)–O(1)	2.324(2)
Dy(1)–O(2)	2.269(3)	Dy(1)–O(2)	2.277(2)
Dy(1)–O(3)	2.356(3)	Dy(1)–O(3)	2.325(2)
Dy(1)–O(4)	2.280(3)	Dy(1)–O(4)	2.355(2)
Dy(1)–O(5)	2.326(3)	Dy(1)–O(5)	2.317(2)
Dy(1)–O(6)	2.318(3)	Dy(1)–O(6)	2.308(2)
Dy(1)–O(7)	2.516(4)	Dy(1)–N(1)	2.308(2)
Dy(1)–O(8)	2.552(4)	Dy(1)–N(2)	2.308(2)
O(2)-Dy(1)-O(1)	73.17(11)	O(2)-Dy(1)-O(1)	73.30(7)
O(3)-Dy(1)-O(1)	78.26(11)	O(3)-Dy(1)-O(1)	79.45(8)
O(4)-Dy(1)-O(1)	116.31(11)	O(4)-Dy(1)-O(1)	141.37(7)
O(5)-Dy(1)-O(1)	144.49(10)	O(3)-Dy(1)-O(2)	84.71(8)
O(6)-Dy(1)-O(1)	82.75(11)	O(3)-Dy(1)-O(6)	150.94(8)
O(4)-Dy(1)-O(2)	79.65(11)	O(4)-Dy(1)-O(5)	141.70(7)
O(4)-Dy(1)-O(3)	71.74(10)	O(1)-Dy(1)-O(5)	76.58(8)
O(2)-Dy(1)-O(3)	124.28(11)	O(3)-Dy(1)-O(5)	136.72(8)
O(4)-Dy(1)-O(5)	80.21(11)	O(4)-Dy(1)-O(2)	78.51(8)
O(2)-Dy(1)-O(5)	79.98(12)	O(3)-Dy(1)-O(2)	84.71(8)
O(2)-Dy(1)-O(6)	84.98(12)	O(6)-Dy(1)-O(2)	79.46(8)
O(3)-Dy(1)-O(6)	137.25(10)	O(5)-Dy(1)-O(2)	121.08(8)

	3	**4**
Dy(1)–O(1)	2.270(2)	2.306(4)
Dy(1)–O(2)	2.311(3)	2.271(4)
Dy(1)–O(3)	2.319(3)	2.327(4)
Dy(1)–O(4)	2.291(2)	2.330(4)
Dy(1)–O(5)	2.331(3)	2.320(3)
Dy(1)–O(6)	2.334(3)	2.298(4)
Dy(1)–N(1)	2.579(3)	2.613(5)
Dy(1)–N(2)	2.614(3)	2.589(5)
O(2)-Dy(1)-O(1)	73.47(9)	2.298(4)
O(3)-Dy(1)-O(1)	121.75(10)	140.73(13)
O(4)-Dy(1)-O(1)	79.87(10)	78.27(14)
O(3)-Dy(1)-O(2)	76.78(10)	79.04(14)
O(3)-Dy(1)-O(6)	136.27(10)	81.77(13)
O(4)-Dy(1)-O(5)	82.00(10)	135.92(13)
O(1)-Dy(1)-O(5)	79.90(10)	77.35(13)
O(3)-Dy(1)-O(5)	141.20(9)	141.76(13)
O(4)-Dy(1)-O(2)	118.47(10)	84.91(14)
O(3)-Dy(1)-O(2)	76.78(10)	79.04(14)
O(6)-Dy(1)-O(2)	78.57(10)	79.96(13)
O(5)-Dy(1)-O(2)	141.93(10)	121.49(14)

Table S2. The selected bond lengths (Å) for reported analogs.

Complexes	Dy–O_1	Dy–O_2	Dy–O_3	Dy–O_4	Dy–O_5	Dy–O_6
$Dy(hafc)_3(bpy)$[1]	2.325(4)	2.314(4)	2.359(4)	2.354(4)	2.356(4)	2.354(4)
$Dy(TFI)_3(bpy)$[2]	2.315(6)	2.363(6)	2.328(6)	2.311(6)	2.359(6)	2.346(5)
$Dy(TTA)_3(bpy)$[3]	2.337(4)	2.297(4)	2.313(4)	2.346(4)	2.321(4)	2.342(4)
$Dy(acac)_3(phen)$[4]	2.321(3)	2.309(3)	2.318(3)	2.335(3)	2.331(3)	2.324(3)
$Dy(TFI)_3(phen)$[2]	2.376(3)	2.315(3)	2.312(3)	2.347(3)	2.352(3)	2.312(3)
$Dy(TTA)_3(phen)$[3]	2.331(5)	2.319(5)	2.315(5)	2.346(5)	2.308(5)	2.321(5)
$Dy(acac)_3(dpq)$	2.302(7)	2.313(7)	2.313(7)	2.319(7)	2.331(7)	2.375(7)
$Dy(acac)_3(dppz)$	2.291(13)	2.313(12)	2.313(12)	2.316(12)	2.325(12)	2.349(13)

Table S3 The mononuclear dysprosium complexes based on β-diketonate ligands and auxiliary ligands behaving as SIM

Complexes	U_{eff}	External field	coordination geometry	Reference
$[Dy(hfac)_3(H_2O)_2]$		No SMM behavior		36
$[Dy(hfac)_3(bpy)]$	38.48 K	0 Oe	D_{2d}	39
$[Dy(TFI)_3(H_2O)_2]$		No SMM behavior		14
$[Dy(TFI)_3(bpy)]$	48.8 K	0 Oe	D_{2d}	14
$[Dy(TFI)_3(phen)]$	57.9 K	0 Oe	D_{4d}	14
$[Dy(TTA)_3(bpy)]$	58 K	0 Oe	D_{4d}	46
$[Dy(TTA)_3(phen)]$	85 K	0 Oe	D_{4d}	46
$[Dy(d\text{-}tfc)_3(bpy)]$	37 and 46 K	1000 Oe	unknown	15
$[Dy(l\text{-}tfc)_3(bpy)]$	37 and 49 K	1000 Oe	unknown	15
$[Dy(d\text{-}tfc)_3(phen)]$	31 K	1000 Oe	unknown	15
$[Dy(l\text{-}tfc)_3(phen)]$	25 K	1000 Oe	unknown	15
$[Dy(tfnb)_3(dppz)]$	65 K	0 Oe	D_{4d}	45
$[Dy(EIFD)_3(bpy)]$	28.8 K	0 Oe	D_{4d}	20
$[Dy(EIFD)_3(phen)]$	41.8 K	0 Oe	D_{4d}	20
$[Dy(EIFD)_3(dpq)]$	41.7 K	450 Oe	D_{4d}	20
$[Dy(EIFD)_3(dppz)]$	32.4 K	1500 Oe	D_{4d}	20