Electronic Supplementary Information

Auxiliary Ligands Field Dominated Single-Molecule Magnets of a Series of Indole-Derivative β-diketone Mononuclear Dy(III) Complexes

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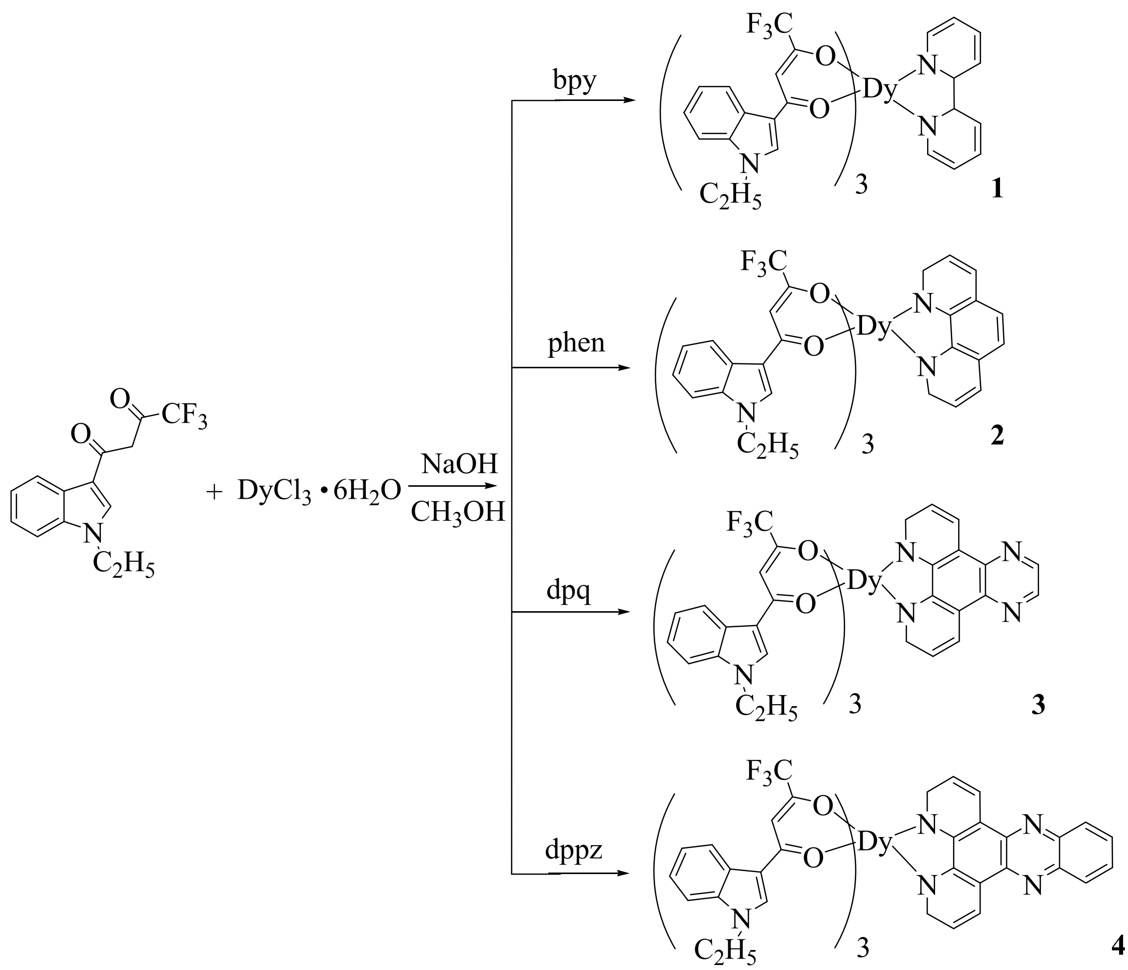

Scheme S1. Synthesis of complexes **1−4**

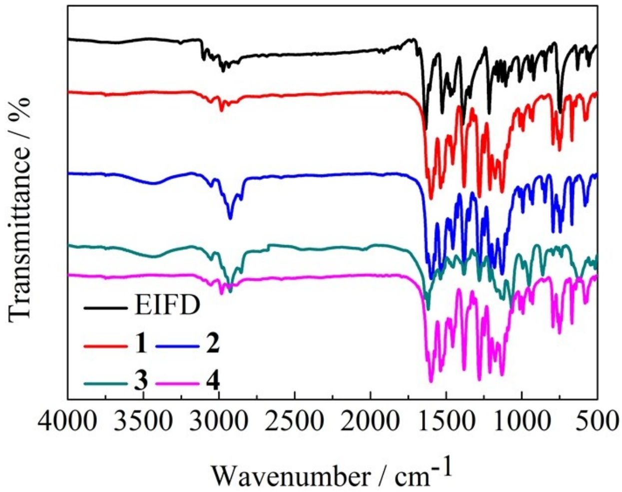

Figure S1. IR spectra of EIFD and complexes **1−4**

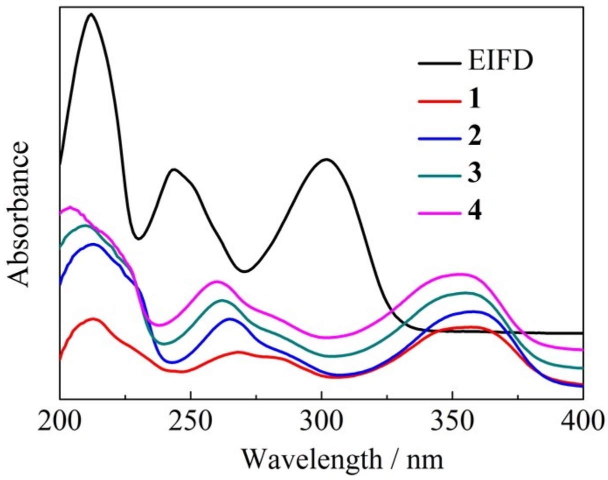

Figure S2. UV absorption spectra of EIFD and complexes **1−4**

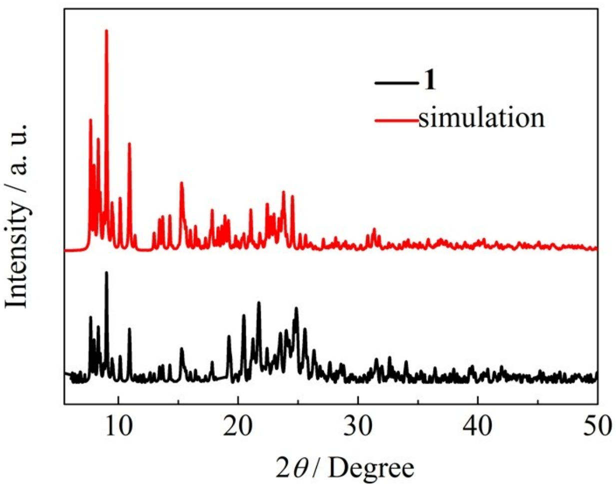

Figure S3. The powder X-ray diffraction patterns and the simulated patterns of complex **1**

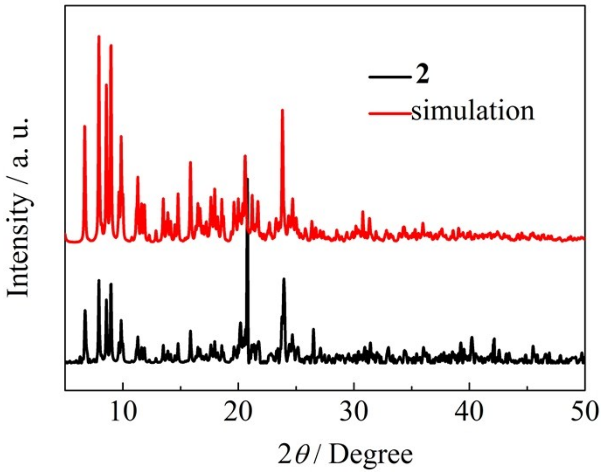

Figure S4. The powder X-ray diffraction patterns and the simulated patterns of complex **2**

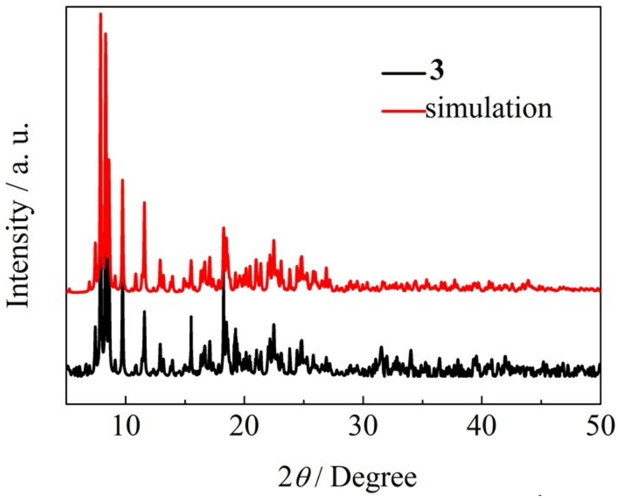

Figure S5. The powder X-ray diffraction patterns and the simulated patterns of complex **3**

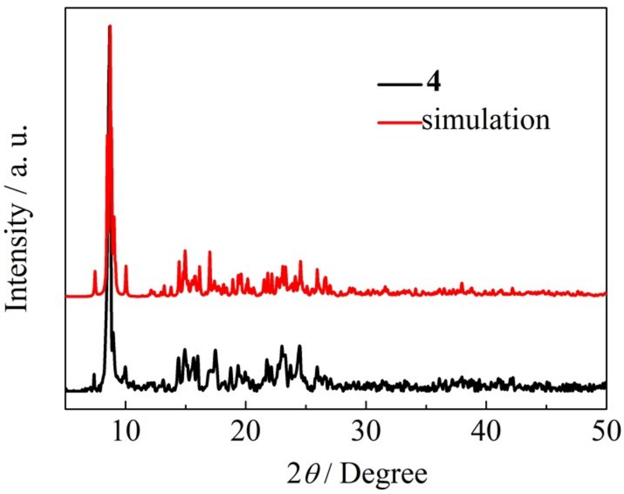

Figure S6. The powder X-ray diffraction patterns and the simulated patterns of complex **4**

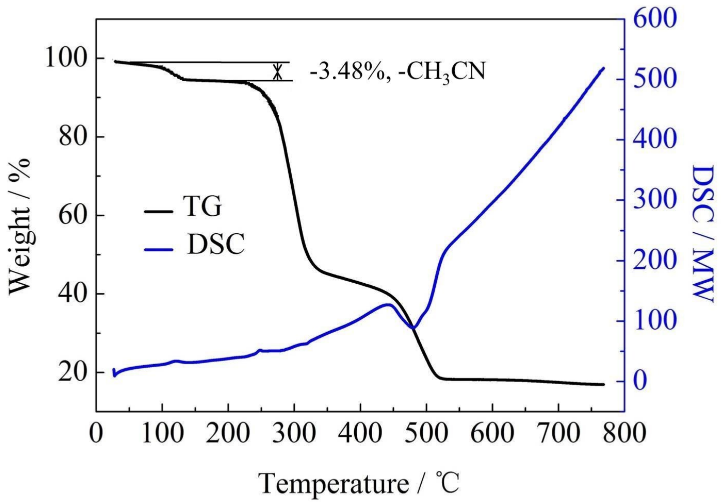

Figure S7. TG-DSC curves of complex **1**

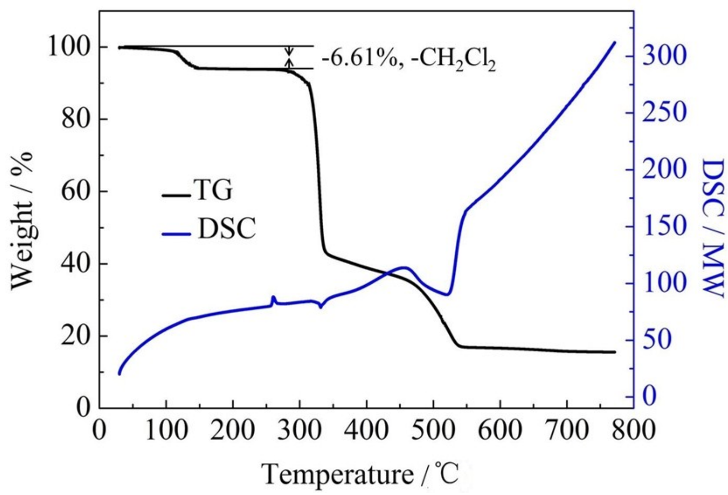

Figure S8. TG-DSC curves of complex **2**

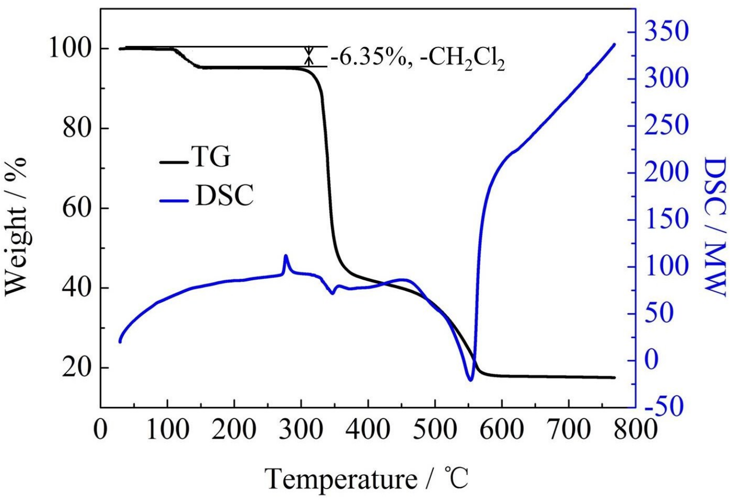

Figure S9. TG-DSC curves of complex **3**

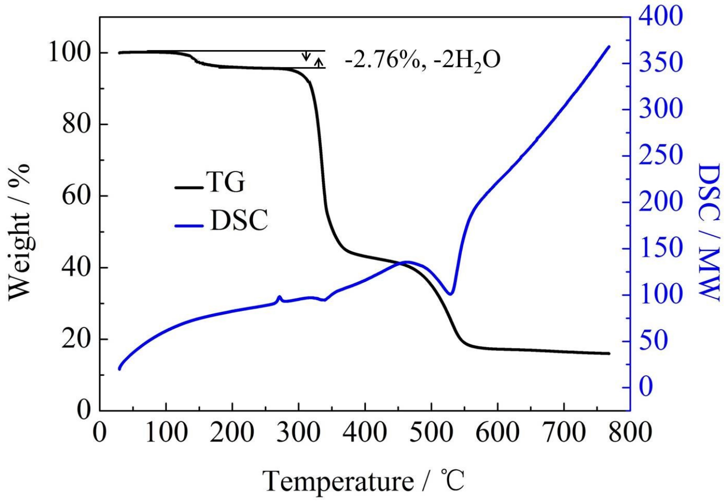

Figure S10. TG-DSC curves of complex **4**

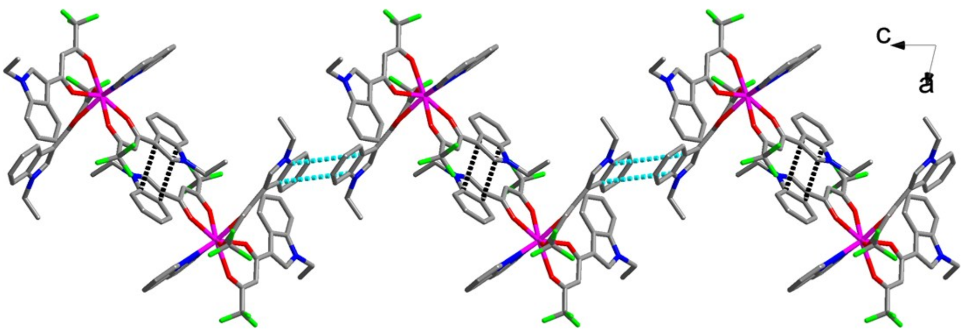

Figure S11. 1D supramolecular chain of complex **1** formed through the π–π interactions between the indole rings

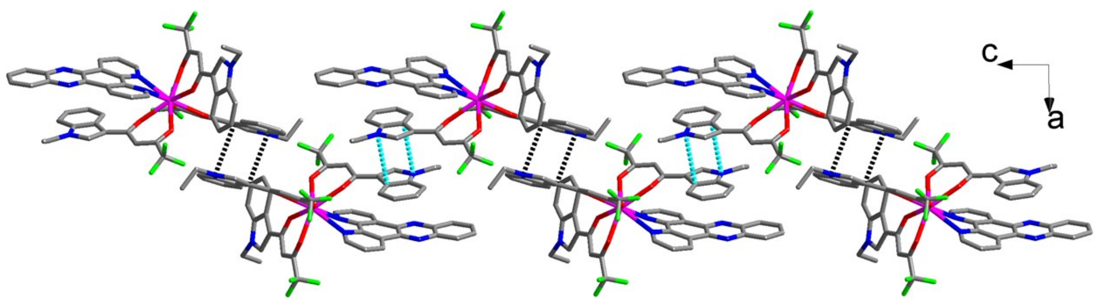

Figure S12. 1D supramolecular chain of complex **4** formed through the π–π interactions between the indole rings

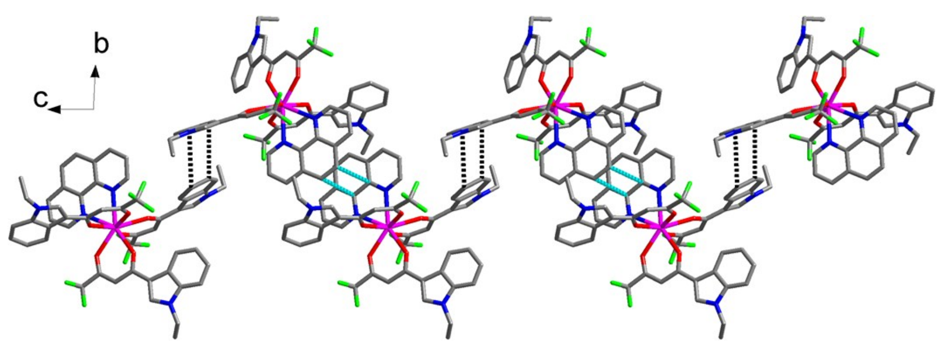

Figure S13. 1D supramolecular chain of complex **2** formed through the π–π interactions between the indole rings as well as between the phen rings

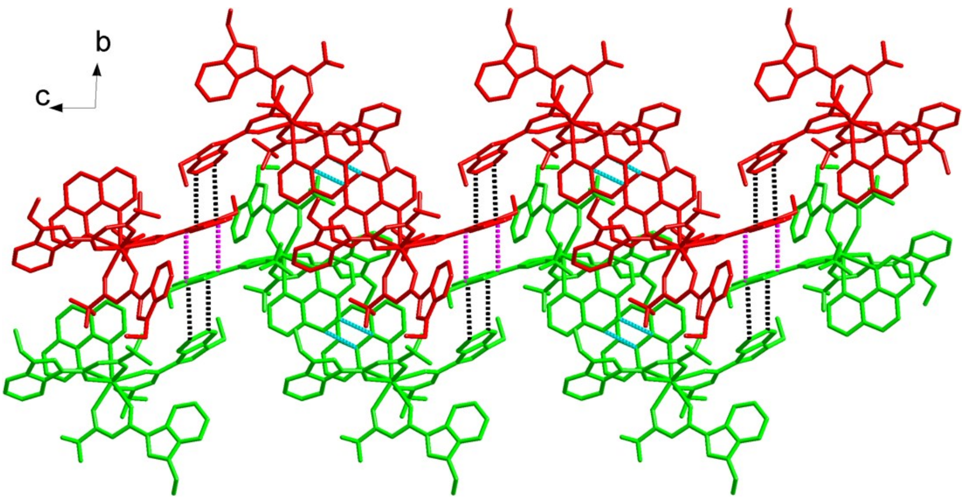

Figure S14. 2D supramolecular layer of complex **2** formed by the π–π interactions between the indole rings

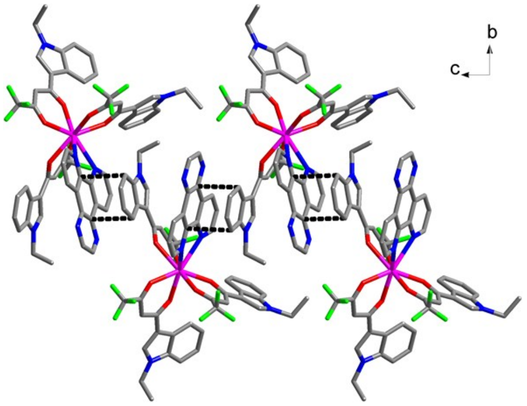

Figure S15. 1D supramolecular chain of complex **3** formed through the π–π interactions between the indole and dpqn rings

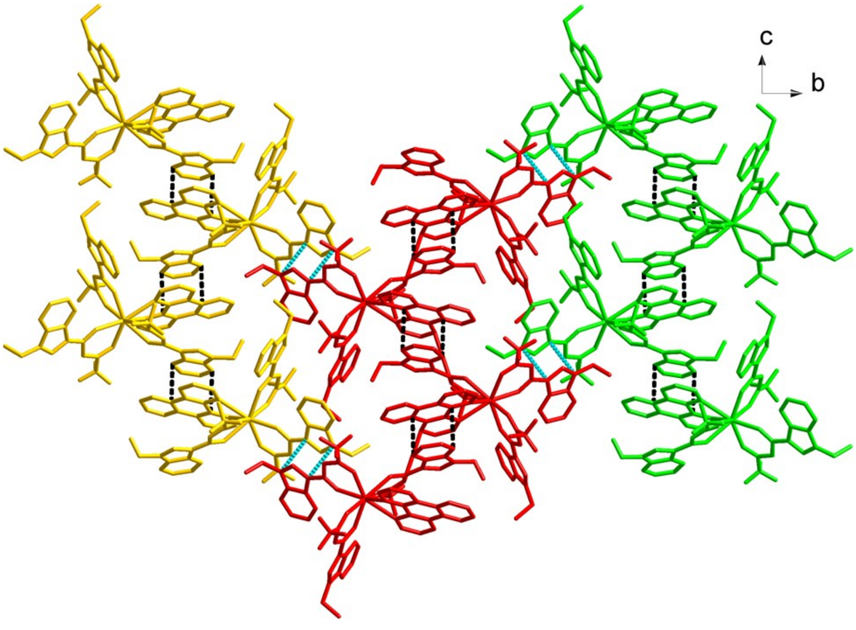

Figure S16. 2D supramolecular layer of complex **3** formed by the π–π interactions between the indole rings

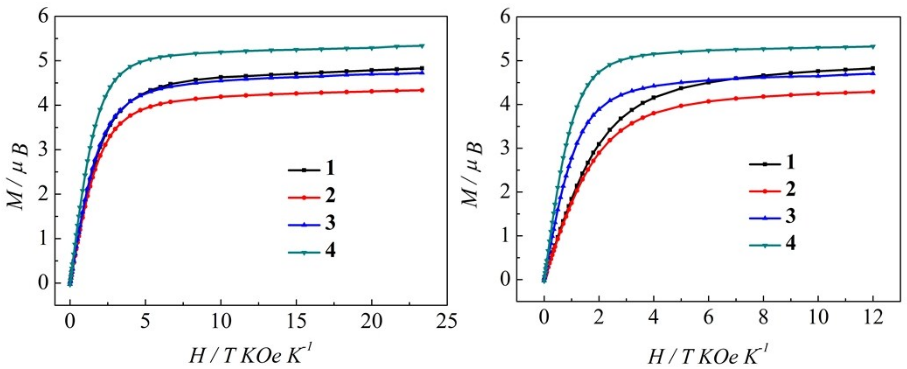

Figure S17. *M vs H / T* data for complexes **1**−**4** at 3 K (left) and 5 K (right)

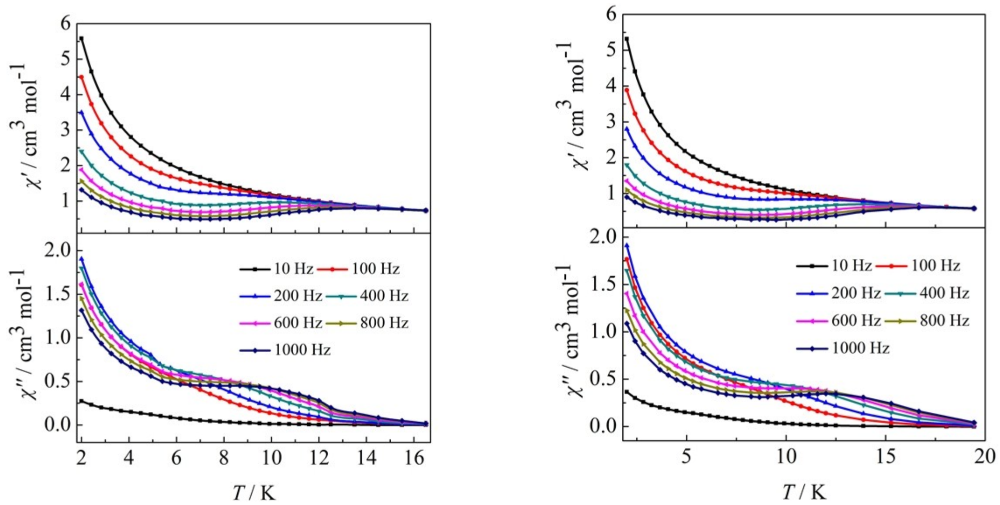

Figure S18. Temperature dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibility of complexes **1** (left) and **2** (right) under 0 Oe in the frequency range 10−1000 Hz

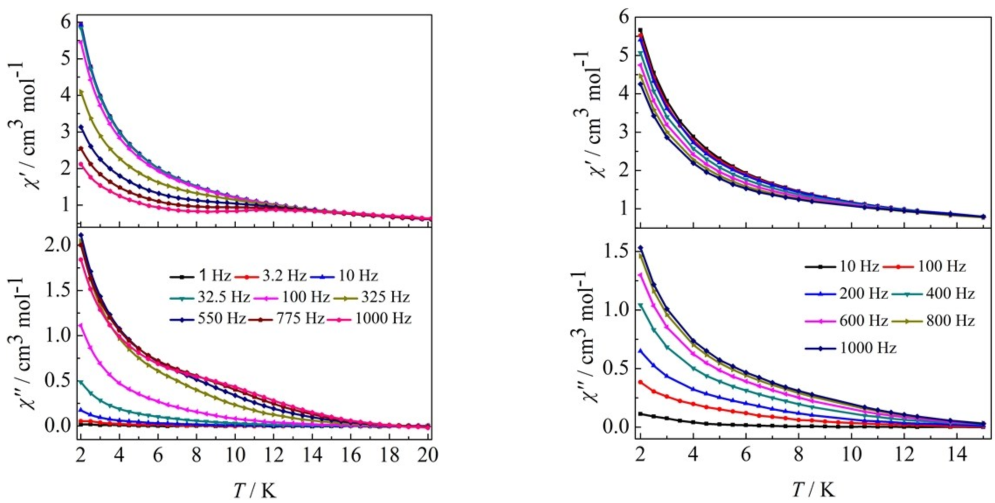

Figure S19. Temperature dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibility of complex **3** under 0 Oe in the frequency range 1−1000 Hz (left) and complex **4** under 0 Oe in the frequency range 10−1000 Hz (right)

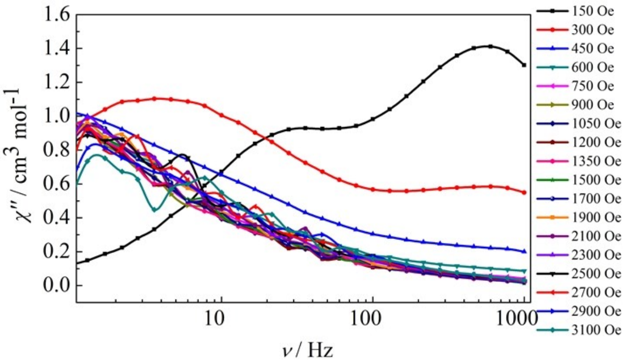

Figure S20. Frequency dependence of the out-of-phase (χ'') ac susceptibility at 2 K in the frequency range 1−1000 Hz and under different field between 150 and 3100 Oe for complex **3**

Table S1. Selected bond lengths and angles for complexes **1−4**

1		**2**		**3**		**4**	
Dy(1)-O(1)	2.329(6)	Dy(1)-O(1)	2.338(3)	Dy(1)-O(1)	2.302(4)	Dy(1)-O(1)	2.344(5)
Dy(1)-O(2)	2.322(5)	Dy(1)-O(2)	2.323(3)	Dy(1)-O(2)	2.306(3)	Dy(1)-O(2)	2.341(5)
Dy(1)-O(3)	2.323(6)	Dy(1)-O(3)	2.313(3)	Dy(1)-O(3)	2.287(3)	Dy(1)-O(3)	2.304(4)
Dy(1)-O(4)	2.327(6)	Dy(1)-O(4)	2.356(3)	Dy(1)-O(4)	2.305(4)	Dy(1)-O(4)	2.299(5)
Dy(1)-O(5)	2.338(7)	Dy(1)-O(5)	2.339(3)	Dy(1)-O(5)	2.342(3)	Dy(1)-O(5)	2.300(5)
Dy(1)-O(6)	2.324(6)	Dy(1)-O(6)	2.344(3)	Dy(1)-O(6)	2.346(3)	Dy(1)-O(6)	2.300(4)
Dy(1)-N(1)	2.580(7)	Dy(1)-N(4)	2.563(3)	Dy(1)-N(4)	2.559(4)	Dy(1)-N(1)	2.587(6)
Dy(1)-N(2)	2.566(7)	Dy(1)-N(5)	2.569(3)	Dy(1)-N(5)	2.589(4)	Dy(1)-N(2)	2.567(6)
O(2)-Dy(1)-O(3)	112.9(2)	O(3)-Dy(1)-O(2)	121.15(11)	O(3)-Dy(1)-O(1)	89.20(14)	O(4)-Dy(1)-O(6)	89.64(17)
O(2)-Dy(1)-O(6)	85.5(2)	O(3)-Dy(1)-O(1)	76.38(11)	O(3)-Dy(1)-O(4)	73.27(13)	O(4)-Dy(1)-O(5)	82.16(19)
O(3)-Dy(1)-O(6)	139.9(2)	O(2)-Dy(1)-O(1)	72.19(10)	O(1)-Dy(1)-O(4)	79.92(14)	O(6)-Dy(1)-O(5)	72.70(16)
O(2)-Dy(1)-O(4)	75.3(2)	O(3)-Dy(1)-O(5)	140.52(11)	O(3)-Dy(1)-O(2)	79.11(13)	O(4)-Dy(1)-O(3)	73.10(16)
O(3)-Dy(1)-O(4)	72.4(2)	O(2)-Dy(1)-O(5)	75.61(10)	O(1)-Dy(1)-O(2)	72.76(13)	O(6)-Dy(1)-O(3)	78.63(16)
O(6)-Dy(1)-O(4)	147.6(2)	O(1)-Dy(1)-O(5)	141.18(10)	O(4)-Dy(1)-O(2)	141.10(13)	O(5)-Dy(1)-O(3)	141.98(19)
O(2)-Dy(1)-O(1)	72.6(2)	O(3)-Dy(1)-O(6)	80.11(11)	O(3)-Dy(1)-O(5)	77.17(13)	O(4)-Dy(1)-O(2)	138.15(17)
O(3)-Dy(1)-O(1)	76.4(2)	O(2)-Dy(1)-O(6)	147.95(11)	O(1)-Dy(1)-O(5)	148.76(13)	O(6)-Dy(1)-O(2)	116.36(18)
O(6)-Dy(1)-O(1)	75.9(2)	O(1)-Dy(1)-O(6)	139.51(10)	O(4)-Dy(1)-O(5)	121.26(14)	O(5)-Dy(1)-O(2)	75.9(2)
O(4)-Dy(1)-O(1)	121.0(2)	O(5)-Dy(1)-O(6)	73.39(10)	O(2)-Dy(1)-O(5)	77.09(12)	O(3)-Dy(1)-O(2)	140.60(19)
O(2)-Dy(1)-O(5)	78.3(2)	O(3)-Dy(1)-O(4)	72.91(11)	O(3)-Dy(1)-O(6)	114.90(13)	O(4)-Dy(1)-O(1)	148.51(16)
O(3)-Dy(1)-O(5)	143.6(2)	O(2)-Dy(1)-O(4)	80.43(11)	O(1)-Dy(1)-O(6)	138.71(13)	O(6)-Dy(1)-O(1)	81.64(16)
O(6)-Dy(1)-O(5)	72.8(2)	O(1)-Dy(1)-O(4)	118.62(11)	O(4)-Dy(1)-O(6)	76.23(13)	O(5)-Dy(1)-O(1)	122.98(18)
O(4)-Dy(1)-O(5)	77.8(2)	O(5)-Dy(1)-O(4)	75.78(11)	O(2)-Dy(1)-O(6)	141.50(12)	O(3)-Dy(1)-O(1)	75.53(16)
O(1)-Dy(1)-O(5)	138.4(2)	O(6)-Dy(1)-O(4)	84.32(10)	O(5)-Dy(1)-O(6)	72.10(12)	O(2)-Dy(1)-O(1)	71.47(17)
O(2)-Dy(1)-N(2)	144.4(2)	O(3)-Dy(1)-N(4)	141.70(12)	O(3)-Dy(1)-N(4)	148.87(14)	O(4)-Dy(1)-N(2)	70.21(18)
O(3)-Dy(1)-N(2)	81.2(2)	O(2)-Dy(1)-N(4)	79.86(11)	O(1)-Dy(1)-N(4)	71.30(14)	O(6)-Dy(1)-N(2)	145.79(19)
O(6)-Dy(1)-N(2)	104.8(2)	O(1)-Dy(1)-N(4)	81.58(12)	O(4)-Dy(1)-N(4)	79.43(14)	O(5)-Dy(1)-N(2)	77.24(19)
O(4)-Dy(1)-N(2)	78.7(2)	O(5)-Dy(1)-N(4)	71.83(12)	O(2)-Dy(1)-N(4)	115.78(14)	O(3)-Dy(1)-N(2)	118.70(18)
O(1)-Dy(1)-N(2)	142.8(2)	O(6)-Dy(1)-N(4)	97.85(11)	O(5)-Dy(1)-N(4)	131.20(13)	O(2)-Dy(1)-N(2)	70.40(19)
O(5)-Dy(1)-N(2)	72.7(3)	O(4)-Dy(1)-N(4)	145.32(12)	O(6)-Dy(1)-N(4)	71.52(13)	O(1)-Dy(1)-N(2)	129.51(18)
O(2)-Dy(1)-N(1)	150.7(2)	O(3)-Dy(1)-N(5)	79.57(11)	O(3)-Dy(1)-N(5)	147.69(14)	O(4)-Dy(1)-N(1)	98.33(18)
O(3)-Dy(1)-N(1)	74.7(2)	O(2)-Dy(1)-N(5)	131.75(11)	O(1)-Dy(1)-N(5)	103.91(14)	O(6)-Dy(1)-N(1)	150.25(17)
O(6)-Dy(1)-N(1)	73.4(2)	O(1)-Dy(1)-N(5)	71.96(11)	O(4)-Dy(1)-N(5)	137.54(14)	O(5)-Dy(1)-N(1)	136.64(17)
O(4)-Dy(1)-N(1)	132.4(2)	O(5)-Dy(1)-N(5)	117.55(11)	O(2)-Dy(1)-N(5)	76.94(14)	O(3)-Dy(1)-N(1)	76.43(17)
O(1)-Dy(1)-N(1)	82.5(2)	O(6)-Dy(1)-N(5)	71.69(11)	O(5)-Dy(1)-N(5)	76.58(13)	O(2)-Dy(1)-N(1)	75.54(18)
O(5)-Dy(1)-N(1)	113.1(2)	O(4)-Dy(1)-N(5)	146.15(11)	O(6)-Dy(1)-N(5)	73.94(14)	O(1)-Dy(1)-N(1)	76.65(17)
N(2)-Dy(1)-N(1)	62.9(2)	N(4)-Dy(1)-N(5)	63.87(11)	N(4)-Dy(1)-N(5)	62.86(14)	N(2)-Dy(1)-N(1)	62.73(19)

Table S2. Fitted parameters of the Cole-Cole plots for complex **1** at H_{dc} = 0 Oe

T/K	χ_S	χ_T	τ	α
2.0	0.55985	5.50312	0.00065	0.16363
2.5	0.44278	4.44845	0.00066	0.16930
3.0	0.37911	3.73436	0.00066	0.17033
3.5	0.30114	3.22051	0.00066	0.18093
4.0	0.25098	2.83365	0.00065	0.18500
4.5	0.24585	2.52765	0.00064	0.18215
5.0	0.23575	2.28348	0.00063	0.17567
5.5	0.23354	2.08575	0.00061	0.16134
6.0	0.22469	1.90868	0.00057	0.14708
6.5	0.23110	1.76715	0.00053	0.13310
7.0	0.22878	1.64533	0.00047	0.11935
7.5	0.22156	1.53607	0.00041	0.10939
8.0	0.19548	1.44310	0.00036	0.10583
9.0	0.19983	1.28474	0.00027	0.09478
10.0	0.19615	1.15743	0.00019	0.09040
11.0	0.23509	1.05425	0.00014	0.09000
12.0	0.17717	1.27314	0.00014	0.10383

Table S3. Fitted parameters of the Cole-Cole plots for complex **2** at H_{dc} = 0 Oe

T/K	χ_S	χ_T	τ	α
2.0	0.33535	5.39061	0.00088	0.16886
2.5	0.24490	4.32805	0.00087	0.17391
3.0	0.15060	3.62311	0.00085	0.18635
3.5	0.17581	3.11314	0.00087	0.17985
4.0	0.15246	2.73553	0.00087	0.18202
4.5	0.15357	2.43680	0.00086	0.17468
5.0	0.13182	2.20117	0.00086	0.17803
5.5	0.11451	2.00705	0.00083	0.17751
6.0	0.08163	1.84865	0.00080	0.18414
6.5	0.12232	1.71037	0.00080	0.16616
7.0	0.10653	1.58709	0.00076	0.15464
7.5	0.08916	1.48660	0.00071	0.15326
8.0	0.11142	1.38946	0.00067	0.12226
9.0	0.06160	1.24244	0.00054	0.13499
10.0	0.06431	1.11911	0.00043	0.11494
11.0	0.06000	1.01511	0.00033	0.09632
12.0	0.07550	0.93646	0.00026	0.09000

Table S4. Fitted parameters of the Cole-Cole plots for complex **3** at H_{dc} = 450 Oe

T/K	χ_S	χ_T	τ	α
5.0	0.24900	2.34959	0.00767	0.20753
5.5	0.22869	2.11283	0.00483	0.16712
6.0	0.20829	1.92396	0.00318	0.13816
6.5	0.18841	1.77153	0.00216	0.11682
7.0	0.17350	1.64238	0.00152	0.09879
7.5	0.15857	1.53140	0.00110	0.08571
8.0	0.14901	1.43453	0.00081	0.07399
9.0	0.13599	1.27631	0.00048	0.05724
10.0	0.13542	1.15014	0.00030	0.04449

Table S5. Fitted parameters of the Cole-Cole plots for complex **4** at H_{dc} = 1500 Oe

T/K	χ_S	χ_T	τ	α
2.0	0.08278	7.43298	0.01395	0.33352
2.5	0.08885	3.91051	0.26244	0.28004
3.0	0.07445	3.14714	0.10160	0.25658
3.5	0.06209	2.67374	0.04420	0.23510
4.0	0.04794	2.38222	0.02255	0.22759
4.5	0.02846	2.17562	0.01256	0.23349
5.0	0.01060	1.99724	0.00736	0.24148
5.5	0.02069	1.84965	0.00464	0.24959
6.0	0.03554	1.72154	0.00305	0.25077
6.5	0.05979	1.60490	0.00210	0.25531
7.0	0.09985	1.50478	0.00149	0.26058
7.5	0.01621	1.41017	0.00107	0.26466
8.0	0.02386	1.32655	0.00079	0.26758
9.0	0.03076	1.19391	0.00045	0.28482
10.0	0.03991	1.08172	0.00027	0.30423
11.0	0.06079	0.99127	0.00017	0.33097
12.0	0.08920	0.91112	0.00010	0.34822