

Electronic Supplementary Information

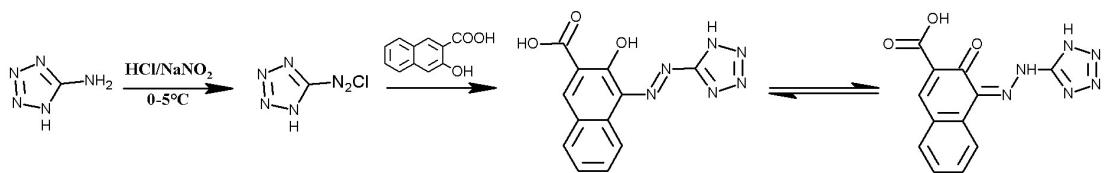
Syntheses, structures and magnetic properties of mononuclear, dinuclear and tetranuclear dysprosium(III) complexes based on azotetrazole-3-hydroxy-2-naphthoic acid

Yun-Jing Zhong^a, Yu-Ying Zhu^a, Jin-Lin Mo^a, Sheng-Lan Ye^a, Wen-Dan Luo^a, Xin Huang, Wen-Bin Chen^{a*} and Wen Dong^{a*}

^aGuangzhou Key Laboratory for Environmentally Functional Materials and Technology, School of Chemistry and Chemical Engineering, Guangzhou University, Guangzhou 510006, P. R. China

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Scheme S1 Synthesis of H₃ATNA

Table S1 geometry analysis by using SHAPE 2.0 program (complex **1**)

	JCSAPR-9 (C _{4v})	CSAPR-9 (C _{4v})	JTCTPR-9 (D _{3h})	TCTPR-9 (D _{3h})	MFF-9 (C _s)
Dy1	2.01041	1.40309	1.65661	1.55637	1.96575

Table S2 geometry analysis by using SHAPE 2.0 program (complex **2**)

	JCSAPR-9 (C _{4v})	CSAPR-9 (C _{4v})	JTCTPR-9 (D _{3h})	TCTPR-9 (D _{3h})	MFF-9 (C _s)
Dy1	3.42932	2.72331	3.67878	2.51046	2.87574
Dy2	SAPR-8 (D _{4d})	TDD-8 (D _{2d})	JBTPR-8 (C _{2v})	BTPR-8 (C _{2v})	JSD-8 (D _{2d})

Table S3 geometry analysis by using SHAPE 2.0 program (complex **3**)

	JCSAPR-9 (C _{4v})	CSAPR-9 (C _{4v})	JTCTPR-9 (D _{3h})	TCTPR-9 (D _{3h})	MFF-9 (C _s)
Dy1	3.31516	2.71549	3.42872	2.40437	2.98622
Dy4	3.18033	2.67698	3.87098	2.87677	2.89240
Dy2	SAPR-8 (D _{4d})	TDD-8 (D _{2d})	JBTPR-8 (C _{2v})	BTPR-8 (C _{2v})	JSD-8 (D _{2d})
Dy3	3.24455	2.38178	2.26877	1.71392	4.53502
	2.52772	1.96188	2.17738	1.55400	4.38655

*CSAPR-9 = Spherical capped square antiprism; TCTPR-9 = Spherical tricapped trigonal prism;

JCSAPR-9 = Capped square antiprism J10; JTCTPR-9 = Tricapped trigonal prism J51;

MFF-9 = Muffin; SAPR-8 = Square antiprism;

TDD-8 = Triangular dodecahedron; JBTPR-8 = Biaugmented trigonal prism J50;

BTPR-8 = Biaugmented trigonal prism; JSD-8 = Snub diphenoïd J84.

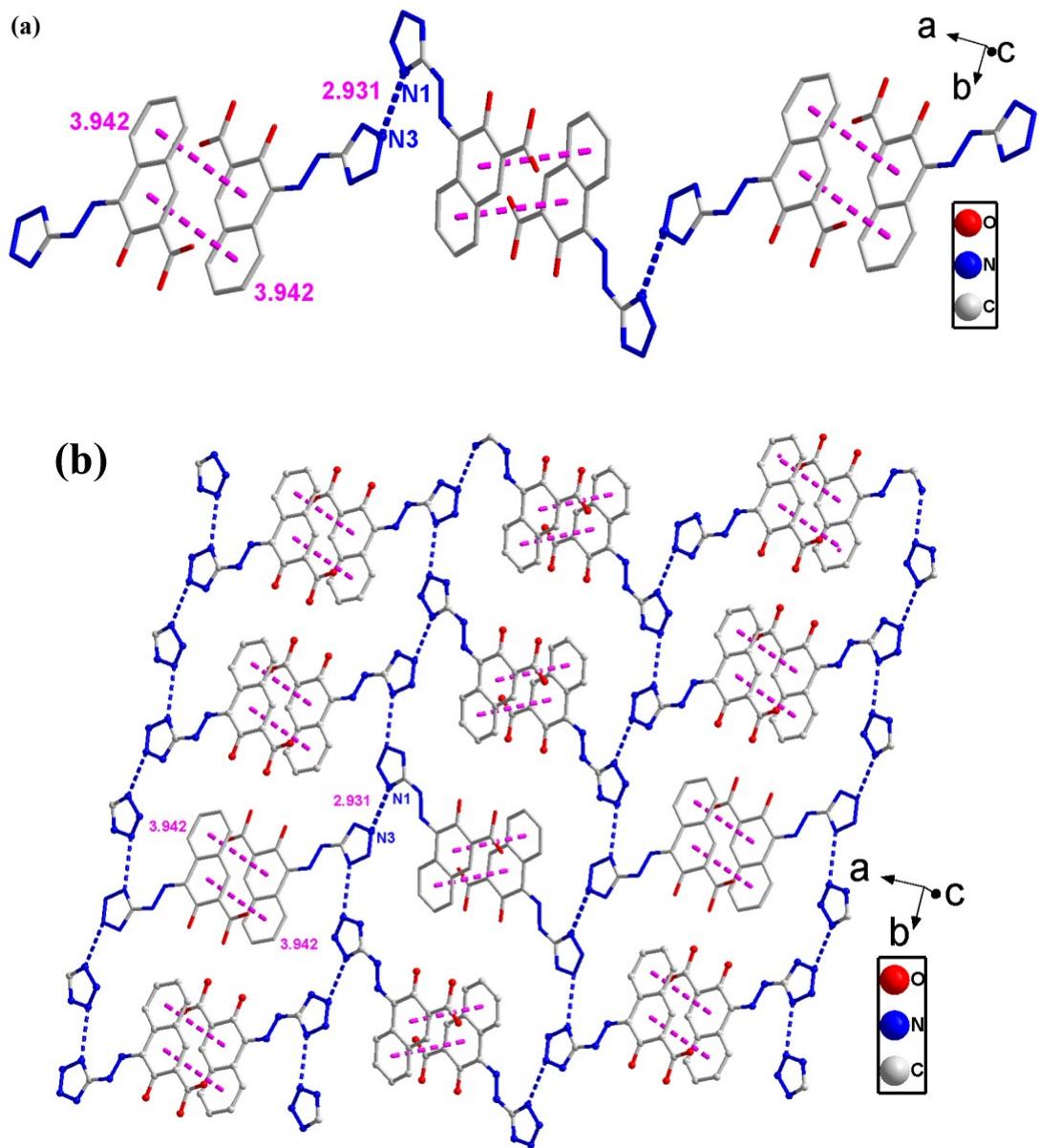


Fig. S1 For H_3ATNA , (a)hydrogen bonds and $\pi-\pi$ stacking interaction along the a axis, (b) hydrogen bonds and $\pi-\pi$ stacking interaction along the a axis and b axis

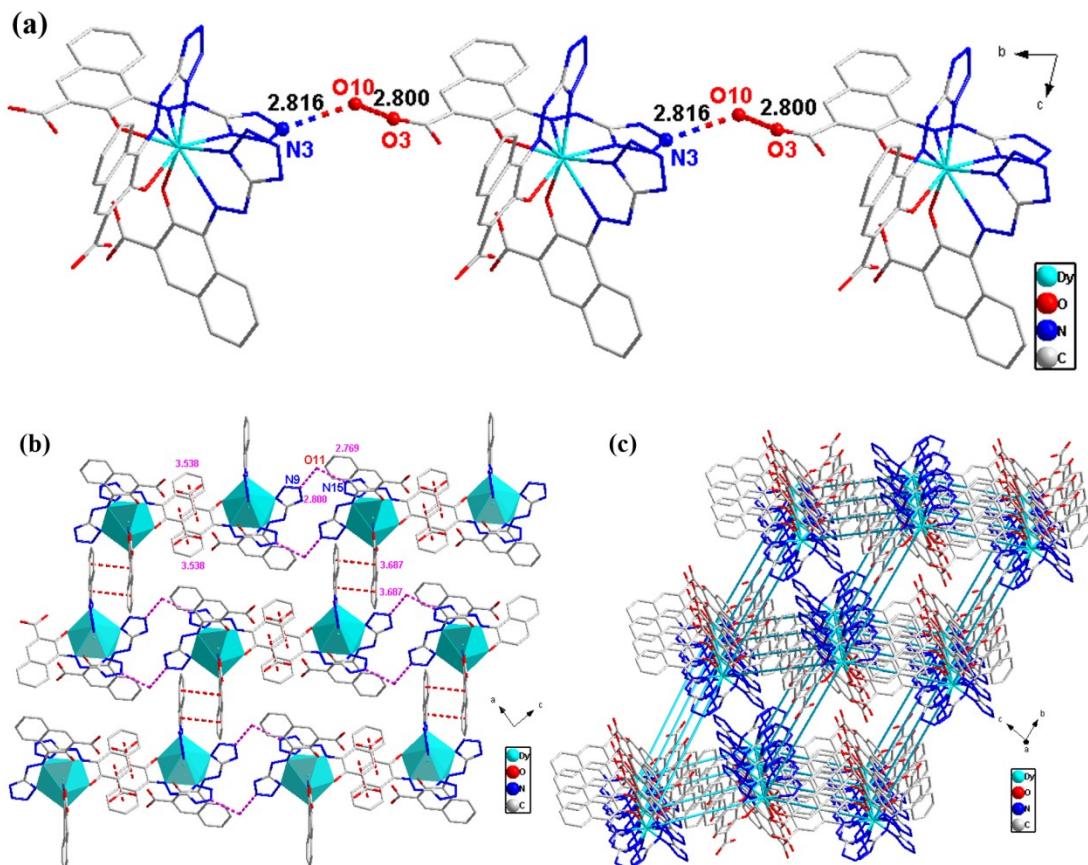


Fig. S2 For **1**, (a)hydrogen bonds along the *b* axis, (b)hydrogen bonds and $\pi-\pi$ stacking interaction along the *a* axis and *c* axis, (c) 3D supramolecular structure(the blue lines between the dysprosium are just for observation, without any interaction).

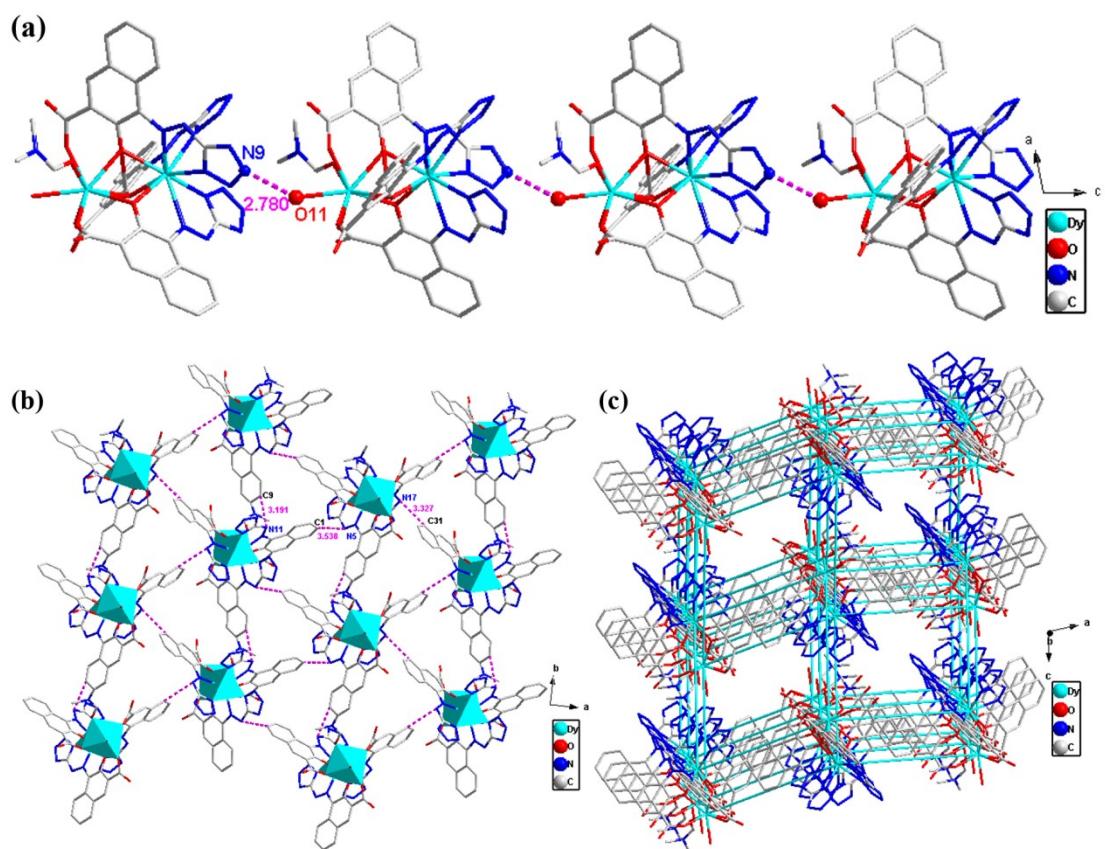


Fig. S3 For **2**, (a) hydrogen bonds along the *c* axis, (b) hydrogen bonds along the *a* and *b* axis to form a two-dimensional plane, (c) 3D supramolecular structure(the blue lines between the dysprosium are just for observation, without any interaction).

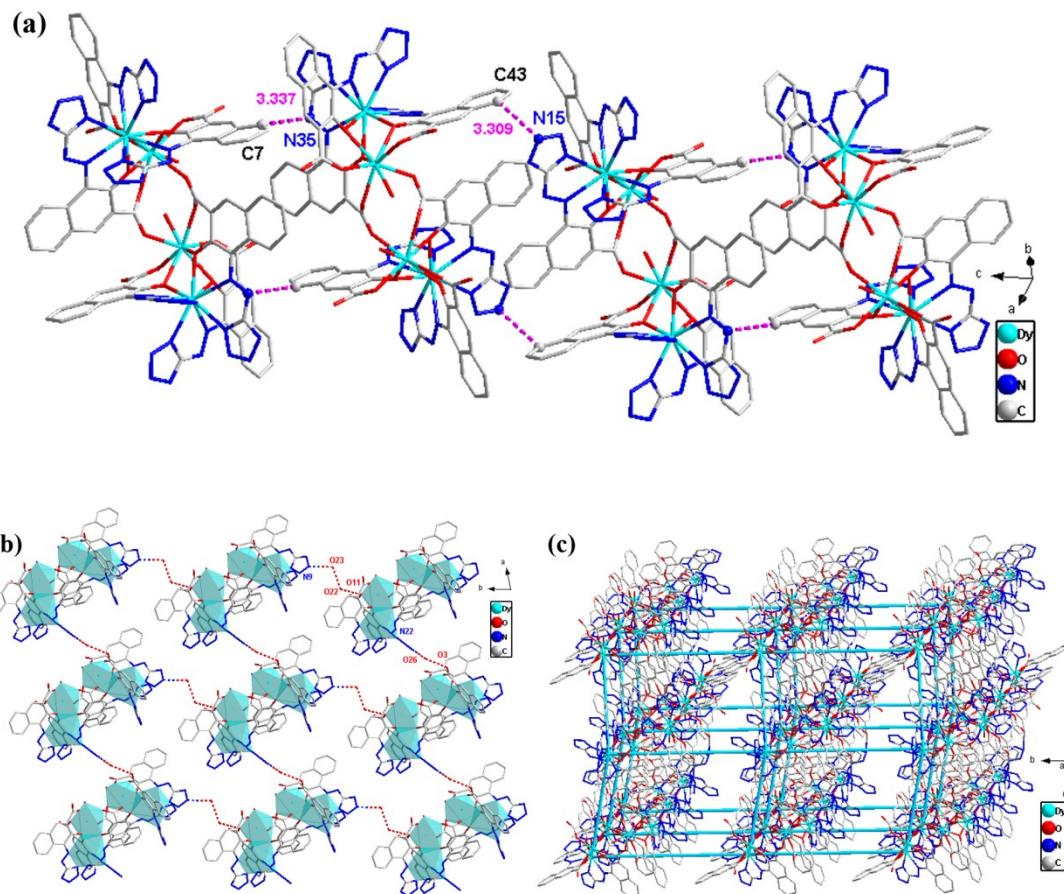


Fig. S4 For 3, (a) hydrogen bonds along the *c* axis, (b) hydrogen bonds along the *a* and *b* axis to form a two-dimensional plane. (c) 3D supramolecular structure(the blue lines between the dysprosium are just for observation, without any interaction).

Table S4 Crystal data and structure refinement of H₃ATNA and complexes **1-3**.

Complexes	H ₃ ATNA	1	2	3
Empirical formula	C ₁₂ H ₈ N ₆ O ₃	C ₅₄ H ₇₆ DyN ₂₁ O ₁₄	C ₄₆ H ₄₇ Dy ₂ N ₂₁ O ₁₆	C ₁₁₅ H ₁₆₅ Dy ₄ N ₄₅ O ₂₉
Formula weight	284.24	1405.85	1475.04	3291.91
Crystal system	monoclinic	triclinic	monoclinic	triclinic
Space group	<i>P</i> 2 ₁ /c	<i>P</i> ī	<i>P</i> 2 ₁ /c	<i>P</i> ī
a/Å	9.4569(11)	13.5498(2)	22.56781(18)	14.5277(2)
b/Å	9.3238(11)	14.6671(2)	12.14163(10)	19.5900(3)
c/Å	13.6224(16)	17.4729(3)	23.5494(2)	24.9631(4)
α/°	90	75.5730(10)	90	85.4820(10)
β/°	106.127(8)	81.5450(10)	101.8928(9)	76.1500(10)
γ/°	90	73.268(2)	90	75.6980(10)
Volume/Å ³	1153.9(2)	3209.98(9)	6314.26(10)	6682.64(18)
Z	4	2	4	2
ρ _{calc} /g·cm ⁻³	1.636	1.455	1.552	1.636
μ/mm ⁻¹	0.124	6.884	13.181	12.505
F (000)	584.0	1450.0	2920.0	3332.0
Reflections collected	18248	44179	49042	94700
Independent reflections	2651	12616	12343	26062
Goodness-of-fit on F ²	1.021	1.067	1.046	1.042
Final R indexes	R ₁ = 0.0394	R ₁ = 0.0476	R ₁ = 0.0502	R ₁ = 0.0707
[I>=2σ (I)]	wR ₂ = 0.0791	wR ₂ = 0.1184	wR ₂ = 0.1259	wR ₂ = 0.1549
Final R indexes	R ₁ = 0.0814	R ₁ = 0.0514	R ₁ = 0.0552	R ₁ = 0.0877
[all data]	wR ₂ = 0.0954	wR ₂ = 0.1201	wR ₂ = 0.1286	wR ₂ = 0.1635
CCDC	2207284	2207285	2207286	2207287

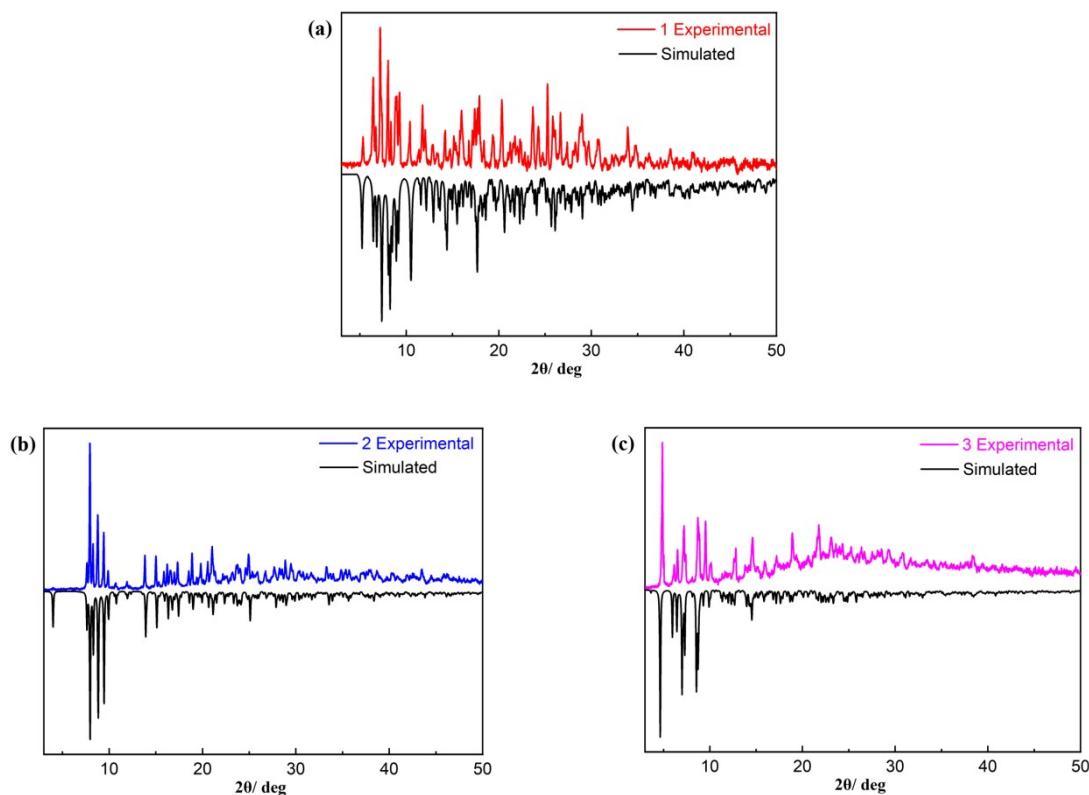


Fig. S5 Powder X-ray diffraction (PXRD) patterns for complexes **1-3**

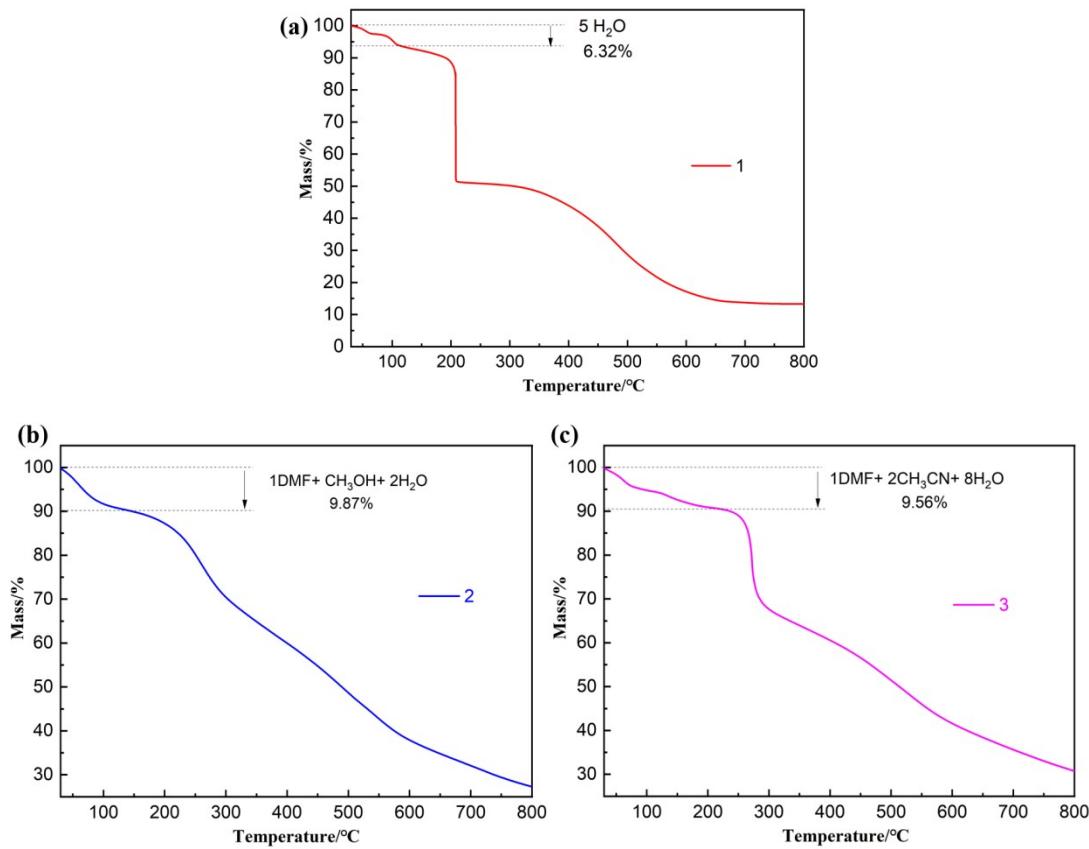


Fig. S6 TG curves of complexes **1-3**.

Table S5 The bond lengths[Å] for H₃ATAN

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C12	1.201(2)	C2	C10	1.462(2)
O2	C12	1.325(2)	C3	C4	1.448(2)
O3	C3	1.2463(19)	C4	C5	1.351(2)
N1	N2	1.3521(18)	C4	C12	1.490(2)
N1	C1	1.330(2)	C5	C11	1.435(2)
N2	N3	1.2885(19)	C6	C7	1.368(3)
N3	N4	1.3617(19)	C6	C11	1.398(2)
N4	C1	1.3137(19)	C7	C8	1.380(3)
N5	N6	1.3277(18)	C8	C9	1.374(2)
N5	C1	1.365(2)	C9	C10	1.391(2)
N6	C2	1.3111(19)	C10	C11	1.404(2)
C2	C3	1.468(2)			

Table S6 The bond angles [°] for complex H₃ATAN

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C1	N1	N2	108.02(14)	C5	C4	C3	120.04(15)
N3	N2	N1	105.87(13)	C5	C4	C12	118.25(16)
N2	N3	N4	111.75(13)	C4	C5	C11	123.77(16)
C1	N4	N3	104.53(13)	C7	C6	C11	120.28(17)
N6	N5	C1	116.44(14)	C6	C7	C8	119.93(19)
C2	N6	N5	120.50(14)	C9	C8	C7	120.78(19)
N1	C1	N5	125.20(15)	C8	C9	C10	120.54(17)
N4	C1	N1	109.83(14)	C9	C10	C2	122.55(15)
N4	C1	N5	124.90(15)	C9	C10	C11	118.56(15)
N6	C2	C3	124.32(15)	C11	C10	C2	118.88(14)
N6	C2	C10	115.70(14)	C6	C11	C5	120.80(15)
C10	C2	C3	119.96(14)	C6	C11	C10	119.90(16)
O3	C3	C2	120.45(15)	C10	C11	C5	119.30(15)
O3	C3	C4	121.84(15)	O1	C12	O2	120.16(19)
C4	C3	C2	117.71(15)	O1	C12	C4	122.50(19)
C3	C4	C12	121.71(16)	O2	C12	C4	117.32(17)

Table S7 The bond lengths[Å] for complex **1**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Dy1	O1	2.331(3)	Dy1	N7	2.438(3)
Dy1	O4	2.306(3)	Dy1	N12	2.622(3)
Dy1	O7	2.310(3)	Dy1	N13	2.454(3)
Dy1	N1	2.455(3)	Dy1	N18	2.604(3)
Dy1	N6	2.582(3)			

Table S8 The bond angles [°] for complex **1**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Dy1	N1	126.82(10)	O4	Dy1	N18	73.47(10)
O1	Dy1	N6	63.93(9)	O7	Dy1	O1	81.06(10)
O1	Dy1	N7	83.44(10)	O7	Dy1	N1	85.58(11)
O1	Dy1	N12	76.17(10)	O7	Dy1	N6	74.63(10)
O1	Dy1	N13	147.81(11)	O7	Dy1	N7	149.50(10)
O1	Dy1	N18	138.36(10)	O7	Dy1	N12	137.10(10)
O4	Dy1	O1	77.17(10)	O7	Dy1	N13	126.09(10)
O4	Dy1	O7	76.32(10)	O7	Dy1	N18	63.84(10)
O4	Dy1	N1	147.47(11)	N1	Dy1	N6	62.89(10)
O4	Dy1	N6	134.16(10)	N1	Dy1	N12	136.93(11)
O4	Dy1	N7	125.25(11)	N1	Dy1	N18	74.32(11)
O4	Dy1	N12	63.50(10)	N6	Dy1	N12	123.90(10)
O4	Dy1	N13	91.82(11)	N6	Dy1	N18	121.60(10)
N7	Dy1	N1	82.94(12)	N13	Dy1	N1	77.19(11)
N7	Dy1	N6	74.98(11)	N13	Dy1	N6	134.00(11)
N7	Dy1	N12	62.27(11)	N13	Dy1	N12	71.88(11)
N7	Dy1	N13	78.48(11)	N13	Dy1	N18	62.37(11)
N7	Dy1	N18	137.94(11)	N18	Dy1	N12	114.48(10)

Table S9 The bond lengths[Å] for complex 2

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Dy1	O4	2.304(3)	Dy1	Dy2	3.6391(4)
Dy1	O7	2.385(3)	Dy2	O4	2.352(3)
Dy1	O1	2.339(3)	Dy2	O7	2.416(3)
Dy1	N7	2.487(4)	Dy2	O1	2.469(3)
Dy1	N12	2.611(4)	Dy2	O5	2.349(4)
Dy1	N6	2.585(4)	Dy2	O2	2.291(4)
Dy1	N13	2.463(4)	Dy2	O10	2.350(4)
Dy1	N18	2.567(4)	Dy2	O8	2.306(4)
Dy1	N1	2.476(4)	Dy2	O11	2.431(4)

Table S10 The bond angles [°] for complex 2

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4	Dy1	Dy2	39.06(8)	O4	Dy2	Dy1	38.13(7)
O4	Dy1	O7	69.77(11)	O4	Dy2	O7	68.47(11)
O4	Dy1	O1	68.10(11)	O4	Dy2	O1	65.24(11)
O4	Dy1	N7	121.54(13)	O4	Dy2	O11	137.56(12)
O4	Dy1	N12	62.35(12)	O7	Dy2	Dy1	40.39(7)
O4	Dy1	N6	82.47(12)	O7	Dy2	O1	65.95(11)
O4	Dy1	N13	151.31(13)	O7	Dy2	O11	147.82(14)
O4	Dy1	N18	132.56(12)	O1	Dy2	Dy1	39.50(8)
O4	Dy1	N1	98.46(13)	O5	Dy2	Dy1	101.26(9)
O7	Dy1	Dy2	41.03(8)	O5	Dy2	O4	68.43(12)
O7	Dy1	N7	93.78(13)	O5	Dy2	O7	136.85(12)
O7	Dy1	N12	89.77(12)	O5	Dy2	O1	97.42(12)
O7	Dy1	N6	131.39(13)	O5	Dy2	O10	77.60(13)
O7	Dy1	N13	122.75(12)	O5	Dy2	O11	71.77(14)
O7	Dy1	N18	63.45(12)	O2	Dy2	Dy1	107.23(10)
O7	Dy1	N1	157.40(13)	O2	Dy2	O4	129.28(13)
O1	Dy1	Dy2	42.15(8)	O2	Dy2	O7	110.66(13)
O1	Dy1	O7	68.50(12)	O2	Dy2	O1	68.86(12)
O1	Dy1	N7	156.49(13)	O2	Dy2	O5	97.96(14)
O1	Dy1	N12	130.22(11)	O2	Dy2	O10	148.16(14)
O1	Dy1	N6	64.28(13)	O2	Dy2	O8	88.56(15)
O1	Dy1	N13	91.56(12)	O2	Dy2	O11	70.03(14)
O1	Dy1	N18	87.48(12)	O10	Dy2	Dy1	104.54(10)
O1	Dy1	N1	126.27(14)	O10	Dy2	O4	78.93(12)
N7	Dy1	Dy2	130.22(10)	O10	Dy2	O7	92.33(13)

N7	Dy1	N12	61.93(13)	O10	Dy2	O1	142.74(12)
N7	Dy1	N6	134.80(14)	O10	Dy2	O11	78.77(15)
N7	Dy1	N18	70.35(14)	O8	Dy2	Dy1	112.33(10)
N12	Dy1	Dy2	92.21(8)	O8	Dy2	O4	132.70(13)
N6	Dy1	Dy2	93.24(10)	O8	Dy2	O7	72.15(12)
N6	Dy1	N12	112.01(13)	O8	Dy2	O1	119.48(12)
N13	Dy1	Dy2	131.74(10)	O8	Dy2	O5	142.16(13)
N13	Dy1	N7	85.19(14)	O8	Dy2	O10	77.54(15)
N13	Dy1	N12	136.03(13)	O8	Dy2	O11	75.73(15)
N13	Dy1	N6	70.20(13)	O11	Dy2	Dy1	171.67(12)
N13	Dy1	N18	62.54(13)	O11	Dy2	O1	135.34(14)
N13	Dy1	N1	76.89(13)	N1	Dy1	N7	75.65(15)
N18	Dy1	Dy2	95.98(9)	N1	Dy1	N12	67.64(13)
N18	Dy1	N12	123.00(13)	N1	Dy1	N6	62.42(15)
N18	Dy1	N6	123.62(13)	N1	Dy1	N18	128.15(13)
N1	Dy1	Dy2	135.80(10)				

Table S11 The bond lengths[Å] for complex 3

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Dy1	Dy2	3.6124(6)	Dy3	Dy4	3.6191(6)
Dy1	O1	2.290(5)	Dy3	O9	2.352(5)
Dy1	O4	2.352(5)	Dy3	O10	2.331(5)
Dy1	O7	2.392(5)	Dy3	O11	2.319(5)
Dy1	N1	2.499(6)	Dy3	O13	2.418(5)
Dy1	N6	2.610(6)	Dy3	O14	2.275(5)
Dy1	N7	2.460(6)	Dy3	O16	2.443(5)
Dy1	N12	2.621(6)	Dy3	O17	2.313(5)
Dy1	N13	2.438(6)	Dy3	O20	2.441(5)
Dy1	N18	2.563(6)	Dy4	O10	2.262(5)
Dy2	O1	2.353(6)	Dy4	O13	2.395(5)
Dy2	O2	2.310(5)	Dy4	O16	2.388(5)
Dy2	O4	2.398(4)	Dy4	N19	2.480(6)
Dy2	O5	2.251(5)	Dy4	N24	2.622(6)
Dy2	O7	2.449(5)	Dy4	N25	2.471(6)
Dy2	O8	2.285(5)	Dy4	N31	2.453(6)
Dy2	O18	2.380(5)	Dy4	N36	2.554(6)
Dy2	O19	2.464(5)	Dy4	N30	2.602(7)

Table S12 The bond angles [°] for complex 3

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Dy1	Dy2	39.56(11)	O1	Dy2	Dy1	38.29(11)
O1	Dy1	O4	68.67(16)	O1	Dy2	O4	66.88(16)
O1	Dy1	O7	72.28(16)	O1	Dy2	O7	70.20(16)
O1	Dy1	N1	122.65(18)	O1	Dy2	O18	74.85(16)
O1	Dy1	N6	62.46(17)	O1	Dy2	O19	131.09(17)
O1	Dy1	N7	88.73(19)	O2	Dy2	Dy1	102.58(12)
O1	Dy1	N12	83.01(17)	O2	Dy2	O1	68.74(17)
O1	Dy1	N13	153.44(19)	O2	Dy2	O4	101.79(17)
O1	Dy1	N18	135.31(17)	O2	Dy2	O7	138.78(16)
O4	Dy1	Dy2	40.97(11)	O2	Dy2	O18	84.73(17)
O4	Dy1	O7	66.07(15)	O2	Dy2	O19	69.75(17)
O4	Dy1	N1	154.56(17)	O4	Dy2	Dy1	40.02(11)
O4	Dy1	N6	129.92(17)	O4	Dy2	O7	64.50(15)
O4	Dy1	N7	121.55(18)	O4	Dy2	O19	147.46(17)
O4	Dy1	N12	62.38(17)	O5	Dy2	Dy1	112.52(14)
O4	Dy1	N13	99.27(18)	O5	Dy2	O1	131.20(18)
O4	Dy1	N18	84.84(17)	O5	Dy2	O2	94.75(19)

O7	Dy1	Dy2	42.33(11)	O5	Dy2	O4	72.78(18)
O7	Dy1	N1	94.38(18)	O5	Dy2	O7	115.18(18)
O7	Dy1	N6	88.73(16)	O5	Dy2	O8	84.51(18)
O7	Dy1	N7	155.72(19)	O5	Dy2	O18	151.74(18)
O7	Dy1	N12	127.97(17)	O5	Dy2	O19	76.63(19)
O7	Dy1	N13	125.83(19)	O7	Dy2	Dy1	41.14(11)
O7	Dy1	N18	64.08(17)	O7	Dy2	O19	141.78(16)
N1	Dy1	Dy2	131.53(14)	O8	Dy2	Dy1	114.20(12)
N1	Dy1	N6	61.71(19)	O8	Dy2	O1	137.37(17)
N1	Dy1	N12	136.89(19)	O8	Dy2	O2	140.49(17)
N1	Dy1	N18	71.52(18)	O8	Dy2	O4	115.43(17)
N6	Dy1	Dy2	91.15(13)	O8	Dy2	O7	73.49(16)
N6	Dy1	N12	119.30(18)	O8	Dy2	O18	78.35(17)
N7	Dy1	Dy2	125.96(15)	O8	Dy2	O19	71.70(17)
N7	Dy1	N1	83.0(2)	O18	Dy2	Dy1	95.06(12)
N7	Dy1	N6	68.72(19)	O18	Dy2	O4	135.07(16)
N7	Dy1	N12	61.81(19)	O18	Dy2	O7	81.32(16)
N7	Dy1	N18	135.9(2)	O18	Dy2	O19	76.72(17)
N12	Dy1	Dy2	90.85(13)	O19	Dy2	Dy1	169.01(13)
N13	Dy1	Dy2	139.17(14)	O10	Dy4	Dy3	38.67(12)
N13	Dy1	N1	78.5(2)	O10	Dy4	O13	67.87(17)
N13	Dy1	N6	129.68(19)	O10	Dy4	O16	72.41(16)
N13	Dy1	N7	77.5(2)	O10	Dy4	N19	121.48(19)
N13	Dy1	N12	70.5(2)	O10	Dy4	N24	62.59(17)
N13	Dy1	N18	62.79(19)	O10	Dy4	N25	86.25(19)
N18	Dy1	Dy2	97.46(12)	O10	Dy4	N31	154.90(19)
N18	Dy1	N6	123.37(18)	O10	Dy4	N36	135.14(18)
N18	Dy1	N12	116.42(18)	O10	Dy4	N30	85.24(19)
O9	Dy3	Dy4	92.26(12)	O13	Dy4	Dy3	41.48(11)
O9	Dy3	O13	133.26(16)	O13	Dy4	N19	153.30(18)
O9	Dy3	O16	79.81(16)	O13	Dy4	N24	129.16(17)
O9	Dy3	O20	78.03(17)	O13	Dy4	N25	119.09(19)
O10	Dy3	Dy4	37.35(11)	O13	Dy4	N31	103.25(19)
O10	Dy3	O9	74.17(16)	O13	Dy4	N36	84.37(18)
O10	Dy3	O13	66.43(16)	O13	Dy4	N30	62.24(18)
O10	Dy3	O16	70.27(16)	O16	Dy4	Dy3	42.08(12)
O10	Dy3	O20	130.52(17)	O16	Dy4	O13	65.40(16)
O11	Dy3	Dy4	100.50(12)	O16	Dy4	N19	92.48(19)
O11	Dy3	O9	90.07(17)	O16	Dy4	N24	88.97(16)
O11	Dy3	O10	68.38(17)	O16	Dy4	N25	154.83(19)

O11	Dy3	O13	97.62(17)	O16	Dy4	N31	126.75(18)
O11	Dy3	O16	138.63(16)	O16	Dy4	N36	64.00(17)
O11	Dy3	O20	71.65(17)	O16	Dy4	N30	127.53(18)
O13	Dy3	Dy4	41.00(11)	N19	Dy4	Dy3	128.45(15)
O13	Dy3	O16	64.22(16)	N19	Dy4	N24	60.91(19)
O13	Dy3	O20	147.91(13)	N19	Dy4	N36	72.0(3)
O14	Dy3	Dy4	112.91(13)	N19	Dy4	N30	138.6(2)
O14	Dy3	O9	153.92(17)	N24	Dy4	Dy3	89.85(12)
O14	Dy3	O10	130.29(17)	N25	Dy4	Dy3	122.76(15)
O14	Dy3	O11	91.82(18)	N25	Dy4	N19	87.4(2)
O14	Dy3	O13	72.17(17)	N25	Dy4	N24	69.00(19)
O14	Dy3	O16	114.43(17)	N25	Dy4	N36	138.6(2)
O14	Dy3	O17	83.34(18)	N25	Dy4	N30	61.5(2)
O14	Dy3	O20	77.91(18)	N31	Dy4	Dy3	143.57(15)
O16	Dy3	Dy4	40.92(11)	N31	Dy4	N19	77.4(2)
O17	Dy3	Dy4	113.56(12)	N31	Dy4	N24	126.57(19)
O17	Dy3	O9	80.22(16)	N31	Dy4	N25	77.7(2)
O17	Dy3	O10	138.15(17)	N31	Dy4	N36	63.14(19)
O17	Dy3	O11	144.78(17)	N31	Dy4	N30	70.2(2)
O17	Dy3	O13	113.71(16)	N36	Dy4	Dy3	97.69(13)
O17	Dy3	O16	73.05(16)	N36	Dy4	N24	124.24(18)
O17	Dy3	O20	73.22(17)	N36	Dy4	N30	112.8(2)
O20	Dy3	Dy4	167.29(12)	N30	Dy4	Dy3	92.54(14)
O20	Dy3	O16	142.15(16)	N30	Dy4	N24	121.95(19)

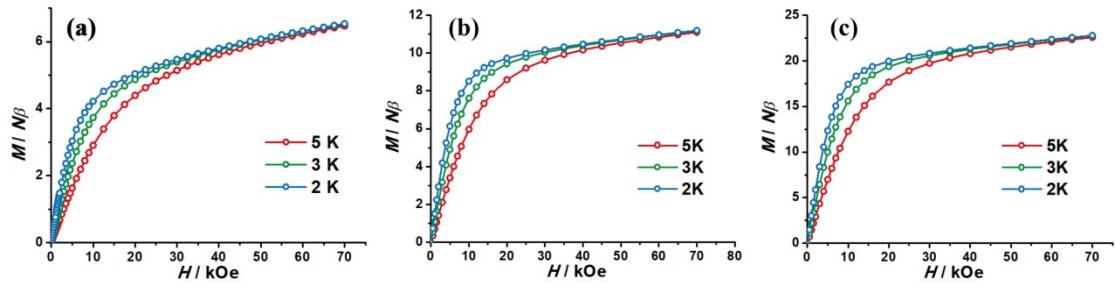


Fig. S7 The isothermal M vs. H plots for **1-3**, respectively.

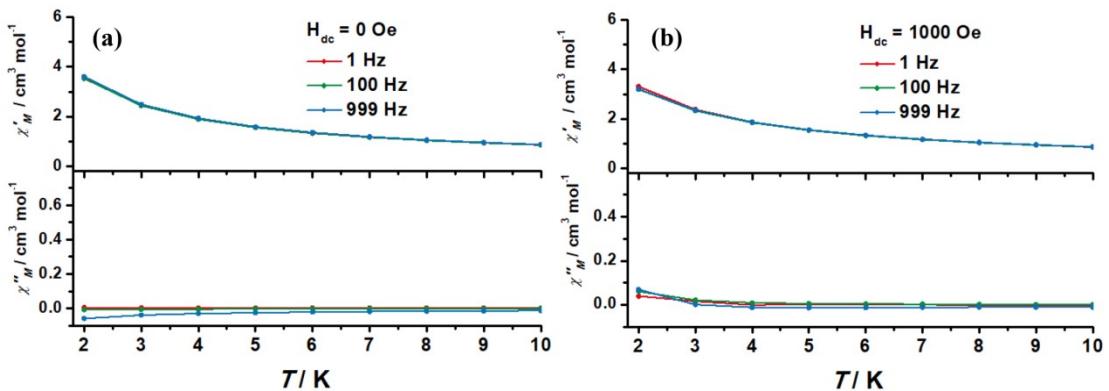


Fig. S8 Temperature dependence of the in-phase χ'_M and out-of-phase χ''_M for **1** in a zero dc field(a); and in a 1000 Oe dc field(b).

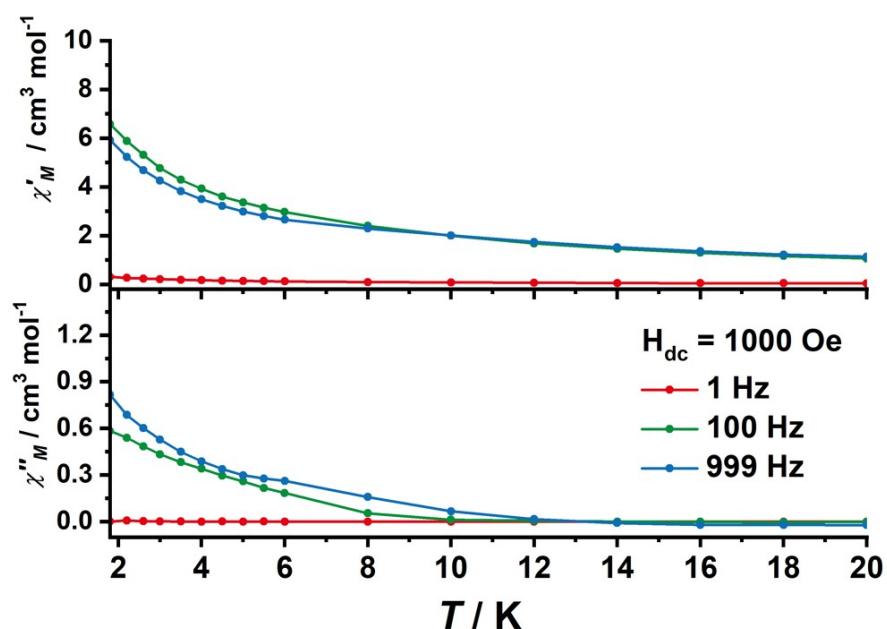


Fig. S9 Temperature dependence of the in-phase χ'_M product and out-of-phase χ''_M for **2** in a 1000 Oe dc field.

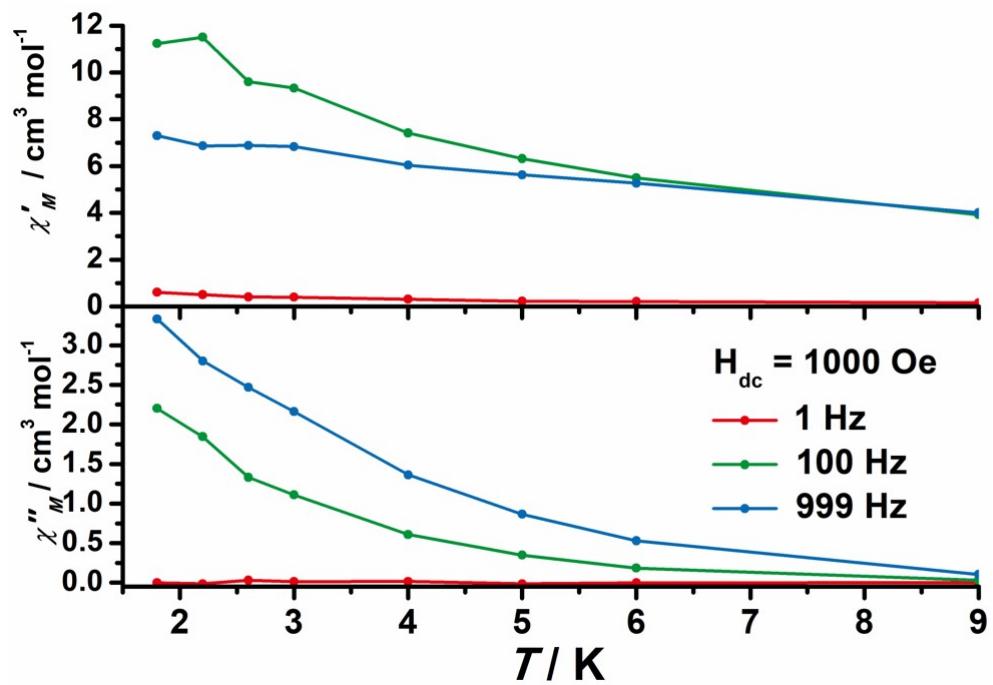


Fig. S10 Temperature dependence of the in-phase χ'_M product and out-of-phase χ''_M for 3 in a 1000 Oe dc field.

Table S13 The average energy barriers($\Delta E/k_B$) and pre-exponential factors(τ_0) of complex **2**

	$\Delta E/k_B$	τ_0
100 Hz	0.81 K	5.5×10^{-5} s
1000 Hz	0.87 K	1.6×10^{-5} s
average	0.84 K	3.6×10^{-5} s

Table S14 The average energy barriers($\Delta E/k_B$) and pre-exponential factors(τ_0) of complex **3**

	$\Delta E/k_B$	τ_0
52 Hz	4.06 K	1.1×10^{-4} s
139 Hz	4.83 K	1.8×10^{-5} s
373 Hz	5.48 K	2.5×10^{-6} s
999 Hz	5.73 K	3.7×10^{-7} s
average	5.03 K	3.3×10^{-5} s