Synthesis, Structures and Magnetic Properties of Butterfly-Shaped Hexanuclear [$Fe^{III}_4Ln^{III}_2$] Single-Molecule Magnets

Supporting Information

Shujing Liu,[a] Chen Zou,[a] Hanjie Wang,[a] Sihuai Chen,*[a] Jun Yuan*[a] and Lihui Jia*[a]

[a] Key Laboratory for Green Chemistry Process of Ministry of Education, School of Chemistry and Environmental Engineering, Wuhan Institute of Technology, Guanggu 1st road 206, Donghu New & High Technology Development Zone, 430073 Wuhan, People's Republic of China. E-mail: sihuai_chen@wit.edu.cn, 380332630@qq.com, jialihui715@wit.edu.cn

Table S1 Crystal data and structure refinement for compounds **1** and **2**.

Compound	**1**	**2**
Formula	$C_{30}H_{72}Y_2Fe_4N_{10}O_{28}$	$C_{30}H_{72}Dy_2Fe_4N_{10}O_{28}$
M_r	1550.36	1697.54
Crystal system	Triclinic	Triclinic
Space group	*P*-1	*P*-1
T (K)	293	296
a (Å)	10.823(3)	11.053(12)
b (Å)	11.181(3)	11.220(12)
c (Å)	12.933(4)	13.170(14)
α (°)	79.54(3)	80.21(3)
β (°)	79.91(2)	80.56(3)
γ (°)	75.82(2)	75.51(3)
V (Å^3)	1478(8)	1546(3)
Z	1	1
D_{calc} (g cm^{-3})	1.742	1.823
F (000)	800	854
μ (mm^{-1})	11.040	3.392
Reflections collected	5016	5420
Unique reflections	5227	5420
Parameters	365	384
R_1 ($I > 2\sigma(I)$)	0.0783	0.0354
wR_2 (all data)	0.2218	0.0632
S (all data)	1.179	1.066

Table S2 Selected bond distances (Å) and angles (deg) for compound **1**.

Bond lengths (Å)					
Y1-Fe1	3.4445(17)	Y1-O9	2.378(7)	Fe1-N3	2.209(9)
Y1-Fe1	3.4760(18)	Y1-O10	2.307(7)	Fe2-O11	1.995(7)
Y1-O2	2.467(8)	Y1-N1	2.879(9)	Fe2-O12	1.924(7)
Y1-O3	2.640(9)	Fe1-Y1	3.4759(18)	Fe2-O13	1.935(7)
Y1-O4	2.455(8)	Fe1-O8	1.967(7)	Fe2-O14	2.003(7)
Y1-O5	2.471(7)	Fe1-O9	2.030(7)	Fe2-N4	2.274(9)
Y1-O7	2.365(7)	Fe1-O10	1.962(7)	Fe2-N5	2.233(9)
Y1-O8	2.276(7)	Fe1-O11	1.993(7)	O9-Y1	2.377(7)
Y1-O9	2.445(7)	Fe1-O14	1.985(7)	O10-Fe1	1.962(7)
Bond angles (deg)					
Fe1-Y1-Fe1	111.62(4)	O9-Y1-O5	125.8(2)	O12-Fe2-O13	147.3(3)
O2-Y1-Fe1	132.98(18)	O9-Y1-O5	141.1(2)	O12-Fe2-O14	109.4(3)
O2-Y1-Fe1	75.81(19)	O9-Y1-O9	72.5(3)	O12-Fe2-N4	79.9(3)
O2-Y1-O3	49.3(2)	O9-Y1-N1	140.1(2)	O12-Fe2-N5	87.8(3)
O2-Y1-O5	67.8(3)	O9-Y1-N1	146.7(2)	O13-Fe2-O11	106.5(3)
O2-Y1-N1	65.9(3)	O10-Y1-Fe1	32.31(18)	O13-Fe2-O14	95.7(3)
O3-Y1-Fe1	83.74(17)	O10-Y1-Fe1	119.95(18)	O13-Fe2-N4	85.2(3)
O3-Y1-Fe1	95.43(19)	O10-Y1-O2	91.5(3)	O13-Fe2-N5	80.6(3)
O3-Y1-N1	93.8(3)	O10-Y1-O3	126.0(3)	O14-Fe2-N4	78.3(3)
O4-Y1-Fe1	140.97(18)	O10-Y1-O4	128.0(2)	O14-Fe2-N5	148.8(3)
O4-Y1-Fe1	106.18(17)	O10-Y1-O5	76.1(2)	N5-Fe2-N4	131.5(3)
O4-Y1-O2	71.5(3)	O10-Y1-O7	82.3(2)	N2-O2-Y1	101.7(6)
O4-Y1-O3	79.1(3)	O10-Y1-O9	84.7(2)	N2-O3-Y1	94.2(6)
O4-Y1-O5	51.9(2)	O10-Y1-O9	65.3(2)	N1-O4-Y1	95.9(6)
O4-Y1-N1	26.0(2)	O10-Y1-N1	102.0(3)	N1-O5-Y1	95.3(6)
O5-Y1-Fe1	96.13(17)	N1-Y1-Fe1	129.60(18)	Y1-O7-H7A	127.4
O5-Y1-Fe1	148.03(18)	N1-Y1-Fe1	118.71(18)	Y1-O7-H7B	126.5
O5-Y1-O3	109.9(2)	Y1-Fe1-Y1	68.38(4)	Fe1-O8-Y1	108.3(3)
O5-Y1-N1	25.9(2)	O8-Fe1-Y1	38.86(19)	C1-O8-Y1	132.0(6)
O7-Y1-Fe1	112.80(18)	O8-Fe1-Y1	103.4(2)	C1-O8-Fe1	115.9(6)
O7-Y1-Fe1	83.18(18)	O8-Fe1-O9	82.3(3)	Y1-O9-Y1	107.5(3)
O7-Y1-O2	138.8(3)	O8-Fe1-O11	160.1(3)	Y1-O9-H9	114.6
O7-Y1-O3	151.6(3)	O8-Fe1-O14	89.9(3)	Y1-O9-H9	114.6
O7-Y1-O4	80.5(3)	O8-Fe1-N3	80.5(3)	Fe1-O9-Y1	103.8(3)
O7-Y1-O5	71.2(2)	O9-Fe1-Y1	41.6(2)	Fe1-O9-Y1	100.2(3)
O7-Y1-O9	72.9(2)	O9-Fe1-Y1	44.3(2)	Fe1-O9-H9	114.6
O7-Y1-O9	134.1(2)	O9-Fe1-N3	148.8(3)	Fe1-O10-Y1	108.7(3)
O7-Y1-N1	75.7(3)	O10-Fe1-Y1	38.9(2)	C5-O10-Y1	132.0(6)
O8-Y1-Fe1	32.82(18)	O10-Fe1-Y1	86.2(2)	C5-O10-Fe1	118.9(6)
O8-Y1-Fe1	139.27(19)	O10-Fe1-O8	103.6(3)	Fe1-O11-Fe2	107.0(3)
O8-Y1-O2	112.9(3)	O10-Fe1-O9	78.6(3)	C6-O11-Fe1	132.2(6)
O8-Y1-O3	68.5(2)	O10-Fe1-O11	93.7(3)	C6-O11-Fe2	119.9(6)

O8-Y1-O4	74.8(2)	O10-Fe1-O14	166.6(3)	C13-O12-Fe2	118.6(7)
O8-Y1-O5	124.3(2)	O10-Fe1-N3	80.4(3)	C10-O13-Fe2	117.7(6)
O8-Y1-O7	87.1(3)	O11-Fe1-Y1	96.3(2)	Fe1-O14-Fe2	107.0(3)
O8-Y1-O9	106.3(2)	O11-Fe1-Y1	155.1(2)	C14-O14-Fe1	133.3(6)
O8-Y1-O9	67.6(2)	O11-Fe1-O9	111.3(3)	C14-O14-Fe2	119.6(6)
O8-Y1-O10	152.3(3)	O11-Fe1-N3	92.7(3)	O4-N1-Y1	58.0(5)
O8-Y1-N1	100.1(3)	O14-Fe1-Y1	138.7(2)	O5-N1-Y1	58.7(5)
O9-Y1-Fe1	35.46(16)	O14-Fe1-Y1	105.0(2)	O6-N1-Y1	174.5(7)
O9-Y1-Fe1	85.84(17)	O14-Fe1-O9	104.2(3)	C2-N3-Fe1	106.1(6)
O9-Y1-Fe1	34.56(17)	O14-Fe1-O11	73.0(3)	C3-N3-Fe1	112.6(6)
O9-Y1-Fe1	84.16(16)	O14-Fe1-N3	101.7(3)	C4-N3-Fe1	104.7(6)
O9-Y1-O2	147.3(3)	N3-Fe1-Y1	118.9(2)	C11-N4-Fe2	113.1(7)
O9-Y1-O2	76.4(3)	N3-Fe1-Y1	111.7(2)	C12-N4-Fe2	104.1(7)
O9-Y1-O3	108.7(2)	O11-Fe2-O14	72.6(3)	C15-N4-Fe2	104.2(7)
O9-Y1-O3	69.6(3)	O11-Fe2-N4	149.5(3)	C8-N5-Fe2	114.7(6)
O9-Y1-O4	134.4(2)	O11-Fe2-N5	78.8(3)	C9-N5-Fe2	104.6(6)
O9-Y1-O4	145.0(3)	O12-Fe2-O11	101.0(3)	C7-N5-Fe2	102.9(6)

Table S3 Selected bond distances (Å) and angles (deg) for compound **2**.

Bond lengths (Å)					
Dy1-Dy1	3.947(3)	Dy1-O9	2.475(5)	Fe2-O6	2.023(3)
Dy1-Fe1	3.477(3)	Dy1-N5	2.904(5)	Fe2-O3	2.015(3)
Dy1-O2	2.286(3)	Dy1-O11	2.764(6)	Fe2-O5	1.935(4)
Dy1-O7	2.415(4)	Fe1-O2	1.984(3)	Fe2-O4	1.927(4)
Dy1-O7	2.459(4)	Fe1-O7	2.043(4)	Fe2-N2	2.253(4)
Dy1-O1	2.314(3)	Fe1-O1	1.988(3)	Fe2-N1	2.299(5)
Dy1-O8	2.399(4)	Fe1-O6	2.010(4)	O7-Dy1	2.415(4)
Dy1-O12	2.485(4)	Fe1-O3	2.001(3)	O1-Dy1	2.314(3)
Dy1-O13	2.484(4)	Fe1-N3	2.222(4)		
Bond angles (deg)					
Fe1-Dy1-Dy1	56.07(6)	O12-Dy1-Dy1	149.16(9)	O5-Fe2-O6	109.49(16)
O2-Dy1-Dy1	85.26(11)	O12-Dy1-Fe1	148.18(9)	O5-Fe2-O3	101.75(15)
O2-Dy1-Fe1	32.68(8)	O12-Dy1-N5	25.83(11)	O5-Fe2-N2	87.49(16)
O2-Dy1-O7	104.70(13)	O12-Dy1-O11	109.31(13)	O5-Fe2-N1	79.44(16)
O2-Dy1-O7	67.57(12)	O13-Dy1-Dy1	159.29(8)	O4-Fe2-O6	96.50(16)
O2-Dy1-O1	152.88(11)	O13-Dy1-Fe1	104.83(10)	O4-Fe2-O3	106.69(16)
O2-Dy1-O8	88.98(13)	O13-Dy1-O12	51.52(11)	O4-Fe2-O5	145.97(15)
O2-Dy1-O12	124.58(13)	O13-Dy1-N5	25.75(11)	O4-Fe2-N2	80.44(16)
O2-Dy1-O13	74.29(13)	O13-Dy1-O11	81.43(15)	O4-Fe2-N1	85.41(16)
O2-Dy1-O9	109.15(14)	O9-Dy1-Dy1	112.53(10)	N2-Fe2-N1	132.23(15)
O2-Dy1-N5	99.74(15)	O9-Dy1-Fe1	130.47(11)	Fe1-O2-Dy1	108.85(15)
O2-Dy1-O11	67.80(12)	O9-Dy1-O12	68.18(13)	C1-O2-Dy1	132.5(3)
O7-Dy1-Dy1	35.54(8)	O9-Dy1-O13	72.31(15)	C1-O2-Fe1	115.8(3)
O7-Dy1-Dy1	36.30(9)	O9-Dy1-N5	66.57(13)	Dy1-O7-Dy1	108.16(14)

O7-Dy1-Fe1	85.36(9)	O9-Dy1-O11	46.87(14)	Dy1-O7-H7	109(4)
O7-Dy1-Fe1	35.27(8)	N5-Dy1-Dy1	174.96(9)	Dy1-O7-H7	125(4)
O7-Dy1-O7	71.84(14)	N5-Dy1-Fe1	128.53(11)	Fe1-O7-Dy1	100.70(15)
O7-Dy1-O12	126.28(11)	O11-Dy1-Dy1	87.89(12)	Fe1-O7-Dy1	103.73(15)
O7-Dy1-O12	142.84(12)	O11-Dy1-Fe1	83.60(10)	Fe1-O7-H7	109(4)
O7-Dy1-O13	146.94(14)	O11-Dy1-N5	94.59(15)	Fe1-O1-Dy1	109.31(15)
O7-Dy1-O13	132.72(12)	O2-Fe1-Dy1	38.47(9)	C5-O1-Dy1	132.4(3)
O7-Dy1-O9	146.37(13)	O2-Fe1-O7	82.00(15)	C5-O1-Fe1	117.9(3)
O7-Dy1-O9	77.20(13)	O2-Fe1-O1	102.82(14)	Fe1-O6-Fe2	106.09(15)
O7-Dy1-N5	141.31(12)	O2-Fe1-O6	90.21(14)	C13-O6-Fe1	133.5(3)
O7-Dy1-N5	146.35(12)	O2-Fe1-O3	161.11(13)	C13-O6-Fe2	120.3(3)
O7-Dy1-O11	107.67(14)	O2-Fe1-N3	80.20(15)	Fe1-O3-Fe2	106.76(14)
O7-Dy1-O11	68.34(14)	O7-Fe1-Dy1	44.03(10)	C6-O3-Fe1	132.5(3)
O1-Dy1-Dy1	72.09(10)	O7-Fe1-N3	148.84(15)	C6-O3-Fe2	119.5(3)
O1-Dy1-Fe1	120.37(8)	O1-Fe1-Dy1	86.99(10)	N5-O12-Dy1	95.8(3)
O1-Dy1-O7	85.31(12)	O1-Fe1-O7	78.43(14)	C12-O5-Fe2	118.8(3)
O1-Dy1-O7	65.21(13)	O1-Fe1-O6	166.96(13)	C9-O4-Fe2	118.0(3)
O1-Dy1-O8	82.44(14)	O1-Fe1-O3	93.42(13)	N5-O13-Dy1	95.9(3)
O1-Dy1-O12	77.07(12)	O1-Fe1-N3	80.86(15)	C3-N3-Fe1	113.6(3)
O1-Dy1-O13	128.48(12)	O6-Fe1-Dy1	103.84(10)	C4-N3-Fe1	103.4(3)
O1-Dy1-O9	93.55(14)	O6-Fe1-O7	104.20(15)	C2-N3-Fe1	105.9(3)
O1-Dy1-N5	102.91(14)	O6-e1-N3	101.24(16)	C18-N2-Fe2	104.3(3)
O1-Dy1-O11	124.35(13)	O3-Fe1-Dy1	154.45(10)	C10-N2-Fe2	104.4(3)
O8-Dy1-Dy1	104.03(10)	O3-Fe1-O7	111.07(15)	C8-N2-Fe2	114.7(3)
O8-Dy1-Fe1	83.44(10)	O3-Fe1-O6	73.66(13)	N4-O9-Dy1	105.7(3)
O8-Dy1-O7	73.26(13)	O3-Fe1-N3	93.11(15)	O12-N5-Dy1	58.3(2)
O8-Dy1-O7	133.60(13)	N3-Fe1-Dy1	112.13(11)	O13-N5-Dy1	58.3(2)
O8-Dy1-O12	72.17(12)	O6-Fe2-N2	149.11(14)	O14-N5-Dy1	173.8(4)
O8-Dy1-O13	79.31(15)	O6-Fe2-N1	77.50(15)	C11-N1-Fe2	104.1(3)
O8-Dy1-O9	140.01(13)	O3-Fe2-O6	73.11(13)	C14-N1-Fe2	104.1(3)
O8-Dy1-N5	75.56(13)	O3-Fe2-N2	78.36(14)	C15-N1-Fe2	113.0(4)
O8-Dy1-O11	153.15(14)	O3-Fe2-N1	149.20(14)	N4-O11-Dy1	92.5(4)

Table S4 Dysprosium geometry analysis for compound **2** by using SHAPE 2.1 program **(CShM = 2.76362)**.

Point group	Geometry	Polyhedron	Dy
D_{9h}	EP-9	Enneagon	32.219
C_{8v}	OPY-9	Octagonal pyramid	20.958
D_{7h}	HBPY-9	Heptagonal bipyramid	16.157
C_{3v}	JTC-9	Johnson triangular cupola J3	15.190
C_{4v}	JCCU-9	Capped cube J8	6.411
C_{4v}	CCU-9	Spherical-relaxed capped cube	5.150

C_{4v}	JCSAPR-9	Capped square antiprism J10	3.565
C_{4v}	**CSAPR-9**	**Spherical capped square antiprism**	**2.764**
D_{3h}	JTCTPR-9	Tricapped trigonal prism J51	4.587
D_{3h}	TCTPR-9	Spherical tricapped trigonal prism	3.519
C_{3v}	JTDIC-9	Tridiminished icosahedron J63	12.436
C_{2v}	HH-9	Hula-hoop	10.455
C_s	MFF-9	Muffin	3.017

Table S5 Fitting parameters from the least-square fitting of the Cole-Cole plots according to the generalized Debye model for compound **2** at H_{dc} =1000 Oe.

Temperature/K	χs / cm^3 mol^{-1}	χT / cm^3 mol^{-1}	α	R
2.0	0.73	22.08583	0.41298	0.97019
3.0	0.64591	8.63302	0.53314	0.97127
4.0	0.46601	4.71849	0.55234	0.9634
5.0	0.37641	3.67148	0.47877	0.95384
6.0	0.33617	3.07766	0.41873	0.95677
7.0	0.31199	2.66597	0.38389	0.97225
8.0	0.28499	2.35066	0.36957	0.98124
9.0	0.26454	2.1076	0.37458	0.98369
10.0	0.24294	1.90747	0.41128	0.98375
11.0	0.19732	1.74862	0.44236	0.98457
12.0	0.19687	1.61265	0.43303	0.98226
13.0	0.17508	1.50144	0.45777	0.97903
14.0	0.19447	1.40374	0.41117	0.97972
15.0	0.19621	0.31967	0.40134	0.98664
16.0	0.16203	1.24183	0.4211	0.98378
17.0	0.18239	1.17435	0.39101	0.97735
18.0	0.17127	1.11556	0.40802	0.98792
19.0	0.18443	1.06243	0.37012	0.97979
20.0	0.06935	1.00561	0.47234	0.98485

Table S6 Fitting parameters from the least-square fitting of the Cole-Cole plots according to the generalized Debye model for compound **3** at H_{dc} = 0 Oe.

Temperature/K	χs / cm^3 mol^{-1}	χT / cm^3 mol^{-1}	α	R
2.0	0.62835	0.61487	-0.00789	0.99033
3.0	0.62351	0.39893	0.01698	0.99255
4.0	0.56108	0.30107	0.02725	0.94825
5.0	0.44605	0.23558	0.03359	0.95794
6.0	0.36527	0.19514	0.03222	0.97882
7.0	0.32930	0.16814	0.02829	0.99301
8.0	0.31877	0.14896	0.02517	0.98637
9.0	0.30352	0.13446	0.02230	0.98578
10.0	0.30314	0.12414	0.02206	0.98297

Table S7 Comparison of compound **2** and **3** with other relevant clusters reported in literature.

Complex	Coordination geometry of Dy^{III}	U_{eff} / K (H_{dc})	τ_0 / s	ref.
$Fe^{III}_4Dy_2$ [a]	square antiprism	21.4	2.7×10^{-8}	36
$Fe^{III}_4Dy_4$ [b]	square antiprism	No SMM		
$Fe^{III}_4Dy_2$ [c]	square antiprism	(18.4 ± 2.7)	$(1.01 \pm 0.89)\times10^{-7}$	37
$Fe^{III}_4Dy_4$ [d]	bicapped trigonal prism	17.15	4.86×10^{-6}	38
$Fe^{III}_4Dy_2$ [e]	muffin	1.2 (1000 Oe)	7.4×10^{-5}	39
$Fe^{III}_6Dy_2$	muffin	12.2 (1000 Oe)	4.0×10^{-5}	
$Fe^{III}_7Dy_3$	square antiprism	33.4	6.6×10^{-8}	40
Fe^{III}_6Gd	triangular dodecahedron	No SMM		41
Fe_4Dy_2 [f]	8-coordinate, C_1 symmetry	26.2	5.9×10^{-5}	42
$Fe_4Y_{1.83}Dy_{0.17}$	8-coordinate, C_1 symmetry	29.0 (1500 Oe)	8.3×10^{-5}	
$Fe^{III}_4Ln_2$ [g]	square antiprism	No SMM		50
$Fe^{III}_4Er_2$	square antiprism	12.8 (500 Oe)	4.6×10^{-7}	51
$Fe^{III}_4Tb_2$	8-coordinate	(26.4 ± 0.4)	$(1.2 \pm 0.2)10^{-9}$	54
$Fe^{III}_4Dy_2$ [h]	8-coordinate	No SMM		
$Fe^{III}_4Dy_4$ [i]	triangular dodecahedron	9.8	1.5×10^{-7}	57
2	9-coordinate, C_1 symmetry	39.7	1.7×10^{-5}	This work
3	9-coordinate, C_1 symmetry	101.5	5.6×10^{-9}	This work

[a] $Fe^{III}_4Dy_2$: $[Fe_4Dy_2(\mu_3\text{-}OH)_2(n\text{-}bdea)_4(C_6H_5CO_2)_8]\cdot MeCN$

[b] $Fe^{III}_4Dy_2$: $[Fe_4Dy_4(\mu_3\text{-}OH)_4(n\text{-}bdea)_4(O_2CC_6H_4CH_3)_{12}]\cdot MeCN$

[c] $Fe^{III}_4Dy_2$: $[Fe_4Dy_2(OH)_2(N_3)_2(bdea)_4(O_2CCMe_3)_5(H_2O)]NO_3\cdot 2(EtOH)$

[d] $Fe^{III}_4Dy_4$: $[Fe^{III}_4Ln^{III}_4O_2(OH)_4(mosaoH)_4(Piv)_4(N\text{-}mdea)_4(H_2O)_2]$

[e] $Fe^{III}_4Dy_2$: $[Fe_4Dy_2(L1)_2(\mu_4\text{-}O)_2(piv)_4(H_2O)_2(NO_3)_4]\cdot CH_3CN\cdot CH_3OH$ {[2,2-((2-((2-hydroxyethyl)amino)cyclohexyl)azanediyl)bis(ethan-1-ol) (H3L1)}

$Fe^{III}_6Dy_2$: $[Fe_6Dy_2(L1)_2(\mu_4\text{-}O)_2(CH_3COO)_6(OH)_2(H_2O)_2(NO_3)_6]\cdot CH_3CN$

$Fe^{III}_7Dy_3$: $[Dy_3Fe_7(\mu_4\text{-}O)_2(\mu_3\text{-}OH)_2(mdea)_7(\mu\text{-benzoate})_4(N_3)_6]_3\cdot 2H_2O\cdot 7CH_3OH$

Fe^{III}_6Gd : $[Fe_6Ln(\mu_3\text{-}OH)_2(mdea)_6(N_3)_6(NO_3)]$

[f] Fe_4Dy_2 : $[Fe_4Dy_2(\mu_3\text{-}OH)_2(mdea)_6(SCN)_2(NO_3)_2(H_2O)_2]\cdot 4H_2O\cdot 2MeCN$

$Fe_4Y_{1.83}Dy_{0.17}$: $[Fe_4Y_{1.83}Dy_{0.17}(\mu_3\text{-}OH)_2(mdea)_6(SCN)_2(NO_3)_2(H_2O)_2]\cdot 4H_2O\cdot 2MeCN$

[g] $Fe^{III}_4Ln_2$: $[Fe^{III}_4Ln^{III}_2(\mu_4\text{-}O)_2(Hedte)_2(piv)_6(NO_3)_2]\cdot 2MeCN\cdot 2CH_2Cl_2$ {Ln = Tb(**1**), Ho(**2**) and Er(**3**), where Hedte = *N,N,N, N'-tetrakis*-(2-hydroxyethyl)ethylenediamine; piv = pivalic acid}

$Fe^{III}_4Er_2$: $[Fe_4Er_2(\mu_3\text{-}OH)_2(n\text{bdea})_4(C_6H_5COO)_8]\cdot MeCN$

$Fe^{III}_4Tb_2$: $[Fe_4Tb_2(O_2CCMe_3)_6(N_3)_4(Htea)_4]$

[h] $Fe^{III}_4Dy_2$: $[Fe_4Ln_2(O_2CCMe_3)_6(N_3)_4(Htea)_4]\cdot 2CH_2Cl_2$

[i] $Fe^{III}_4Dy_4$: $[\{Fe_4(dea)_4Dy_4(deaH)_8(\mu_2\text{-}OMe)_4\}(NO_3)_4]\cdot 4(H_2O)$

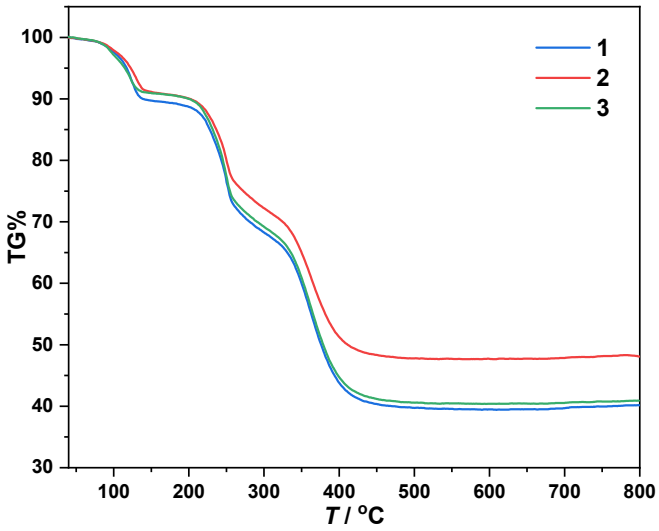

Figure S1. Thermogravimetric curves for **1-3**.

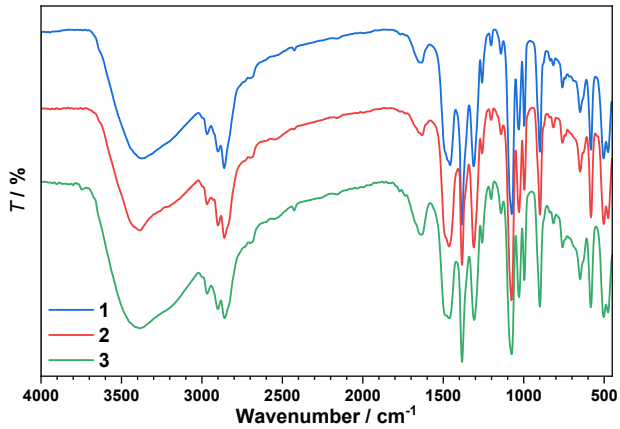

Figure S2. Infrared spectrum for **1-3**.

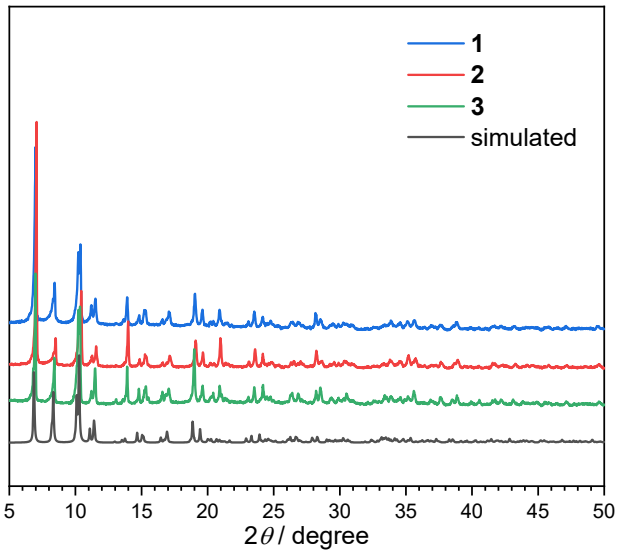

Figure S3. X-ray powder diffraction: measured for compounds **1-3** in comparison with that simulated from the single-crystal structure of compound **2**.

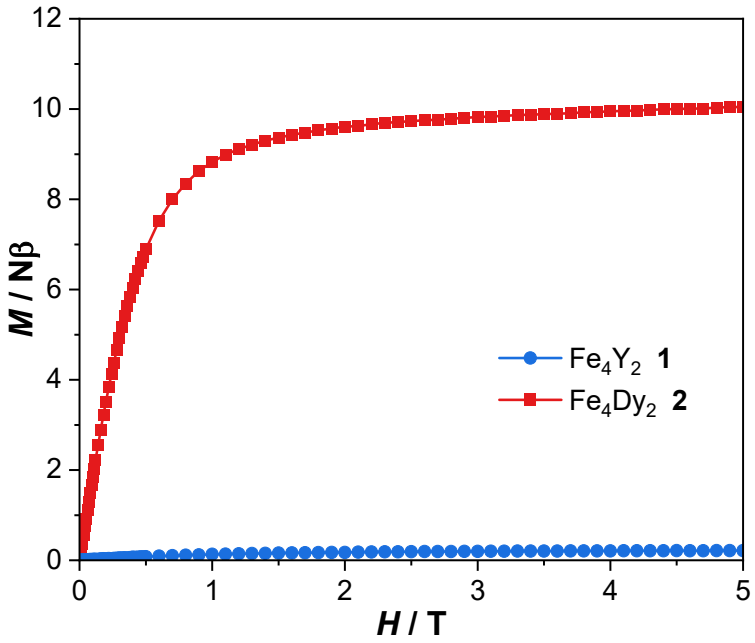

Figure S4. Field dependence of magnetization at 2 K for compounds **1** and **2**.

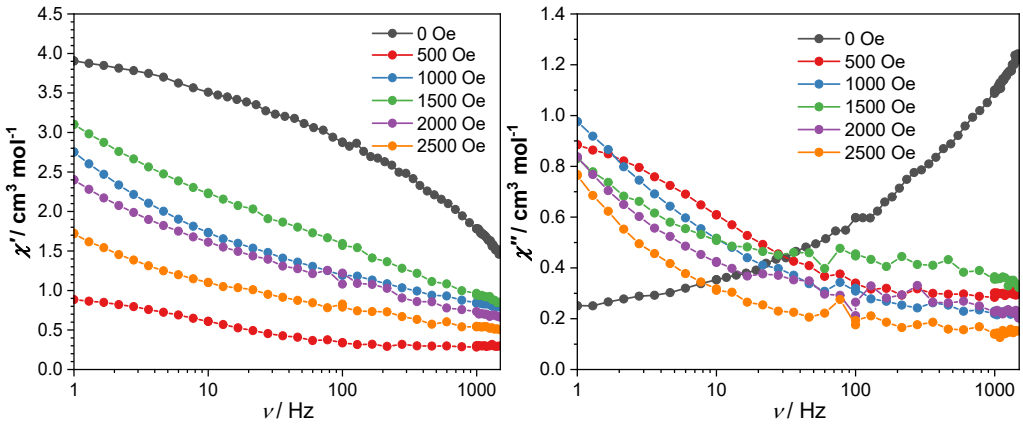

Figure S5. Frequency dependence of the in-phase (χ') (left) and out-of-phase(χ'') (right) ac susceptibility component under indicated dc field at 2 K for **2**.