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SUPPORTING INFORMATION

Synthesis, structures and magnetic properties of four Dysprosium-based complexes with a multidentate ligand with steric constrain

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Solvents mask analyses.

Mask routine of Olex2 (similar to PLATON/QUEEZE) analyses estimate the electron count to be 126 within 734 Å^3 void per cell for **Dy_2**, 70 within 306 Å$_3$ void per cell for **Dy_4** and 280 within 1488 Å$_3$ void per cell for **Dy_6**. Commonly, it is a feasible way to assign the diffuse solvent according to the electrons in the void as reported in ref. [1]. All complexes were obtained in the same solvent system (MeOH−MeCN). The TENTATIVE assignment of the solvents is described in detail as below.

(1) Solvents assignment in Dy_2.

The structure refinement of **Dy_2** with a lower symmetry *P-1* and two formula units in one cell. The residual electron density was treated as diffuse contributions using the mask routine of Olex2 and located a series of voids with 126 electrons per cell, it might be possible that the formula unit includes two CH_3CN molecules (22 e) and one CH_3OH molecules (18 e). These solvent molecules assigned are in line with the result by elemental analysis. The tentative formula is $[Dy_2(H^{py}L)(L)(CH_3COO)]\cdot 2CH_3CN\cdot CH_3OH$ (**$Dy_2\cdot 2CH_3CN\cdot CH_3OH$**).

(2) Solvents assignment in Dy_4.

The structure refinement of **Dy_4** with a lower symmetry *P-1* and one formula unit in one cell. The residual electron density was treated as diffuse contributions using the mask routine of Olex2 and located a series of voids with 70 electrons per cell, it might be possible that the formula unit includes four CH_3OH molecules (72 e). These solvent molecules assigned are in line with the result by elemental analysis. The tentative formula is $[Dy_4(HL)_2(u_3\text{-}OH)_2Cl_6]\cdot 4CH_3OH$ (**$Dy_4\cdot 4CH_3OH$**).

(3) Solvents assignment in Dy_6.

The structure refinement of **Dy_6** with a higher symmetry *Pbca* and four formula units in one cell. The residual electron density was treated as diffuse contributions using the mask routine of Olex2 and located a series of voids with 280 electrons per cell, it might be possible that the formula unit includes four CH_3OH molecules (72 e). These solvent molecules assigned are in line with the result by elemental analysis. The tentative formula is $[Dy_6(L)_2(u_3\text{-}OH)_4(CH_3COO)_8]\cdot 4CH_3OH$ (**$Dy_6\cdot 4CH_3OH$**).

[1] O. V. Dolomanov.; D. B. Cordes.; N. R. Champness.; A. J. Blake.; L. R. Hanton.; G. B. Jameson.; M. Schröder.; C. Wilson. ***Chem. Commun***., 2004, 642.

Crystal Data Warnings and Replies

The B-alerts in **Dy_2**:
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta (Min).
Response: The missing FCF reflections below theta(min) were caused by the high beamstop theta(min) limit set.

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 0.95Ang From C2 2.58 eA^{-3}
Response: This residual density in the structure is likely due to unsuitable absorption correction.

The B-alerts in **Dy_4**:
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).
Response: The missing FCF reflections below theta(min) were caused by the high beamstop theta(min) limit set.

The B-alerts in **Dy_5**:
PLAT420_ALERT_2_B D-H Bond Without Acceptor O8 --H8A.
Response: This problem may arise from the disordered nature of O8 and H8 atoms.

The B-alerts in **Dy_6**:
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).
Response: The missing FCF reflections below theta(min) were caused by the high beamstop theta(min) limit set.

Contents.

Table S1. Crystal Data and Structure Refinement for **Dy_2**, **Dy_4**, **Dy_5** and **Dy_6**.

	Dy_2	**Dy_4**	**Dy_5**	**Dy_6**
Chemical formula	$C_{67}H_{70}Dy_2N_8O_{15}$	$C_{64}H_{76}Cl_6Dy_4N_6O_{18}$	$C_{46}H_{56}Dy_5N_3O_{24}$	$C_{80}H_{100}Dy_6N_6O_{36}$
Formula weight	1554.35	2082.25	1853.97	2704.19
Temperature/K	293	293	100	293
Crystal system	triclinic	triclinic	Monoclinic	orthorhombic
Space group	P**Error!**	P**Error!**	$P2_1/n$	Pbca
a(Å)	14.1814(5)	10.9250(3)	10.9825	22.6360(3)
b(Å)	15.2007(7)	11.2522(4)	22.9575	16.7245(2)
c(Å)	17.7267(6)	16.2537(5)	23.0079	23.9473(3)
α(°)	79.139(3)	96.322(3)	90	90
β(°)	89.186(3)	98.838(2)	98.137(1)	90
γ(°)	64.683(4)	111.745(3)	90	90
V ($Å^3$)	3382.9(3)	1803.23(11)	5742.60 (9)	9065.9(2)
Z	2	1	4	4
ρ_{calcd} (g cm^{-3})	1.4	1.799	2.138	1.82
F (000)	1365	942	3504	4600
Reflection collected	51034	25793	44436	40010
Independent reflections	15096 (Rint = 0.0630)	7361 (Rint = 0.0451)	10117 (Rint = 0.0531)	10761 (Rint = 0.0321)
GOF on F2	1.116	1.052	1.132	1.134
R1a / wR2 b (I > 2σ(I))	0.0626 / 0.1541	0.0375/0.1061	0.0479/0.1204	0.0532/0.1583
R1/ wR2 (all data)	0.1106 / 0.1941	0.0529/0.1181	0.0528/0.1230	0.0731/0.1749
CCDC numbers	2202411	2202419	2204294	2204296

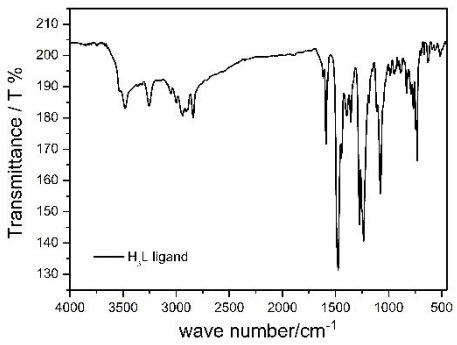

Fig. S1. IR spectrum of H_3L ligand.

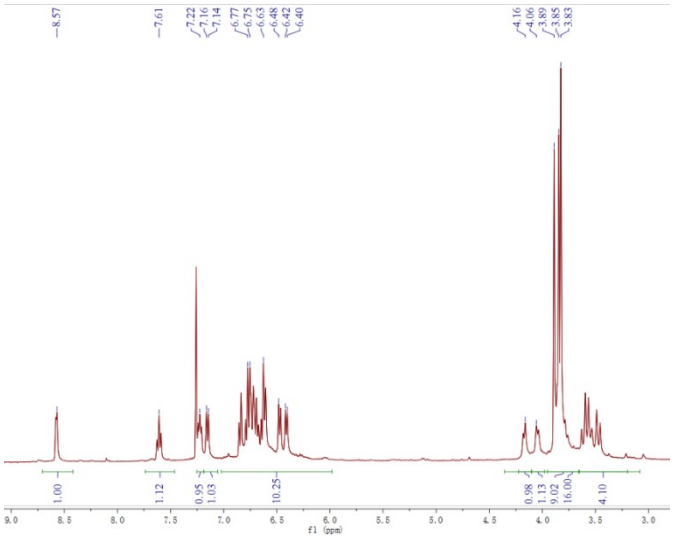

Fig. S2. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of H_3L ligand in DCl_3.

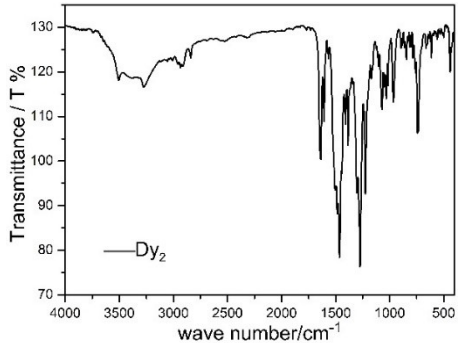

Fig. S3. IR spectrum of **Dy_2**.

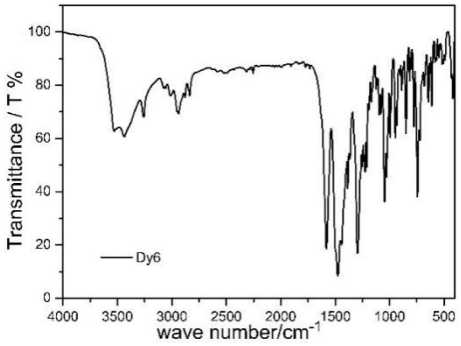

Fig. S4. IR spectrum of **Dy_6**.

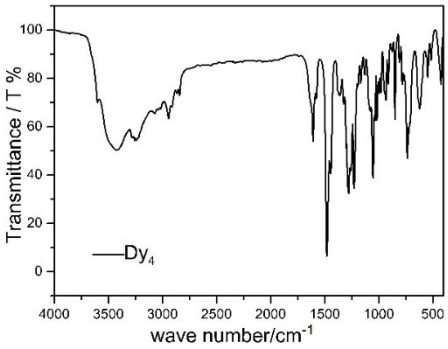

Fig. S5. IR spectrum of **Dy_4**.

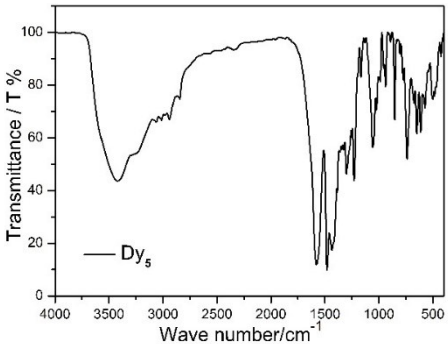

Fig. S6. IR spectrum of **Dy_5**.

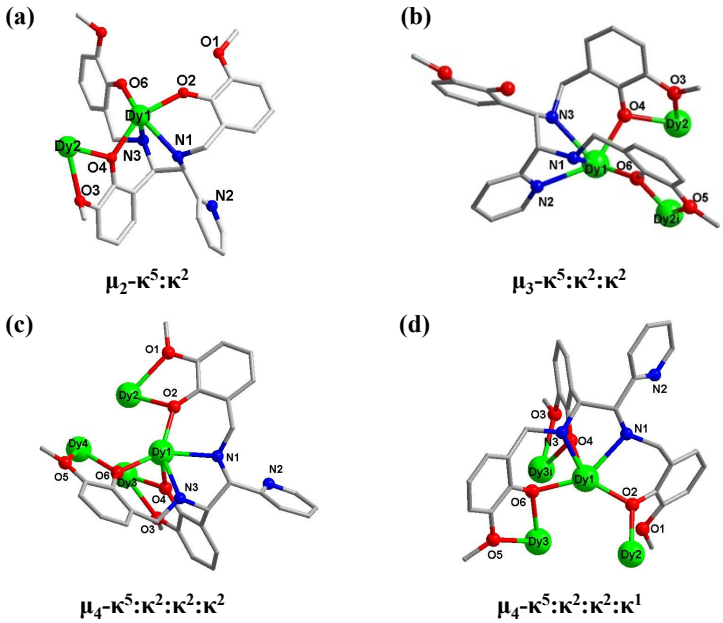

Fig. S7. Different coordination modes of H_3L for complexes: (a) **Dy_2**; (b) **Dy_4**; (c) **Dy_5**; (d) **Dy_6.**

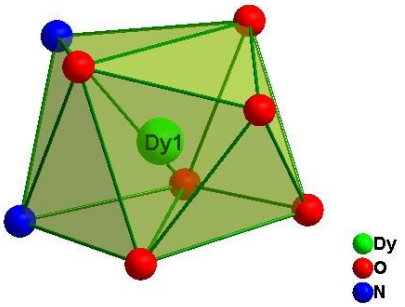

Fig. S8. Coordination polyhedron surrounding of Dy(III) for **Dy_2.**

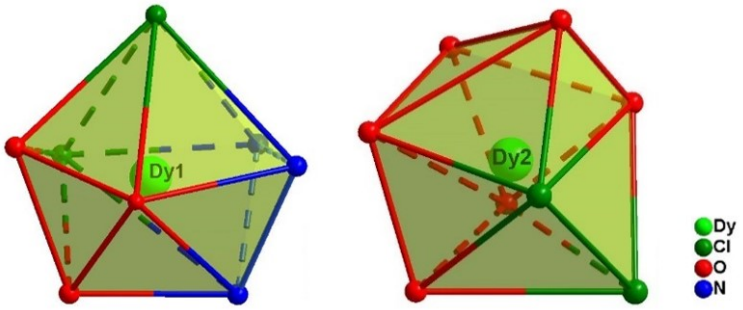

Fig.S9. Coordination polyhedron surrounding of Dy(III) for **Dy_4.**

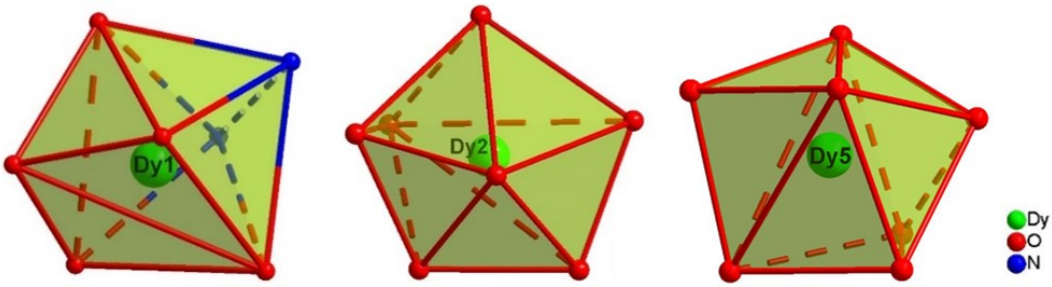

Fig. S10. Coordination polyhedron surrounding of Dy(III) for **Dy_5.**

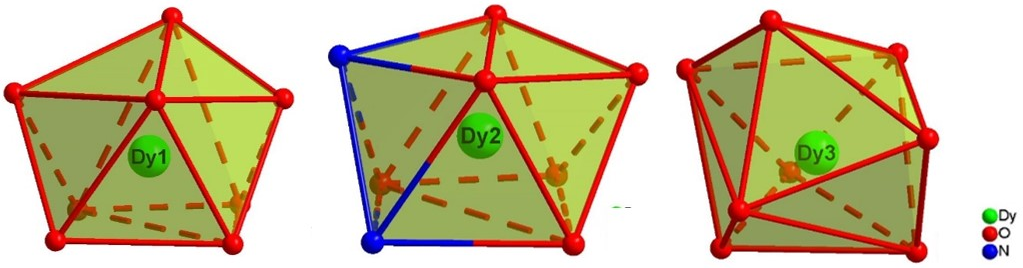

Fig. S11. Coordination polyhedron surrounding of Dy(III) for **Dy_6.**

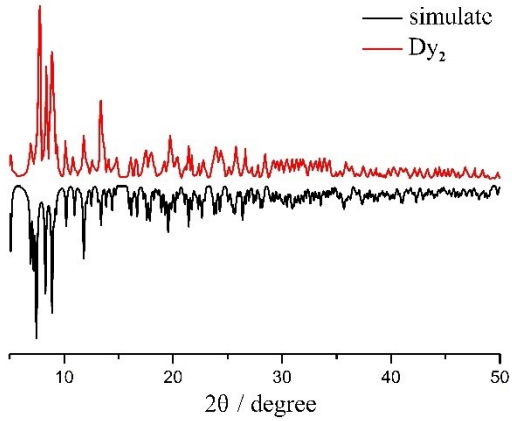

Fig. S12. Powder X-ray diffraction pattern of **Dy_2** at room temperature, together with the calculated pattern from the single crystal data.

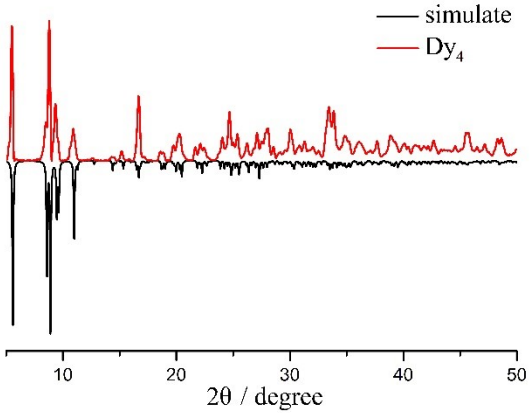

Fig. S13. Powder X-ray diffraction pattern of **Dy_4** at room temperature, together with the calculated pattern from the single crystal data.

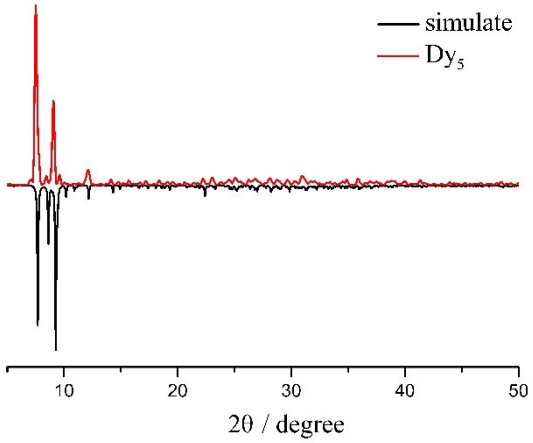

Fig. S14. Powder X-ray diffraction pattern of **Dy_5** at room temperature, together with the calculated pattern from the single crystal data.

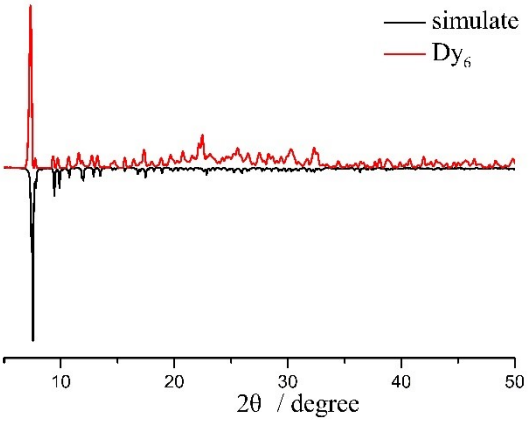

Fig. S15. Powder X-ray diffraction pattern of **Dy_6** at room temperature, together with the calculated pattern from the single crystal data.

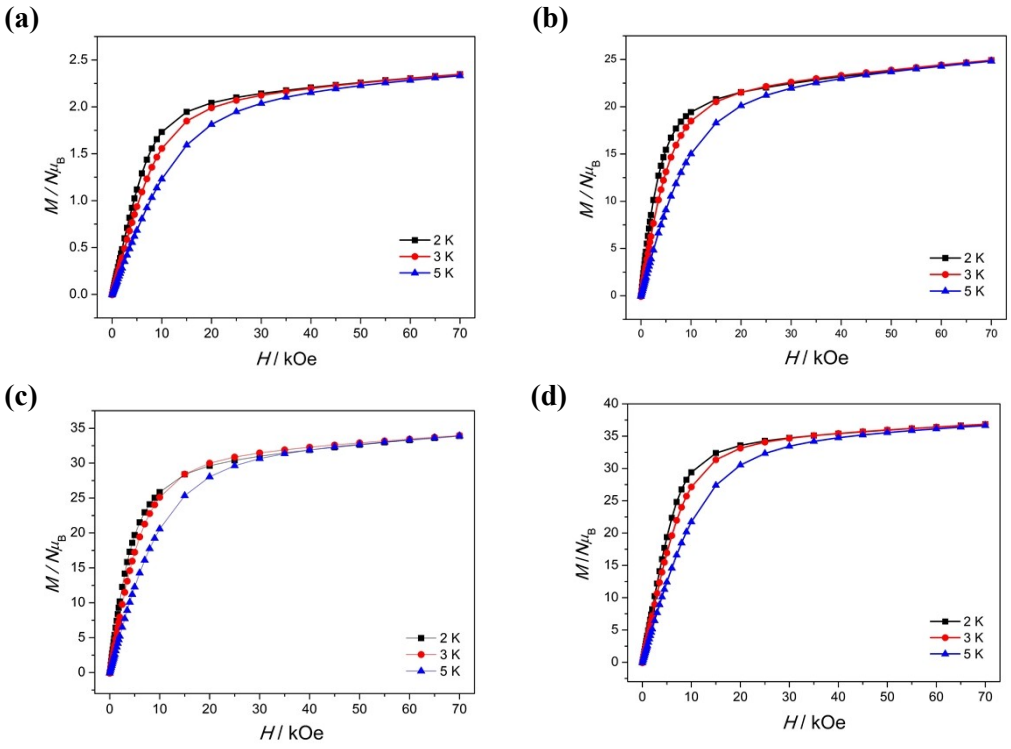

Fig. S16. M versus H plots under different temperatures for **Dy_2**(a); **Dy_4**(b)**; Dy_5**(c) and **Dy_6**(d).

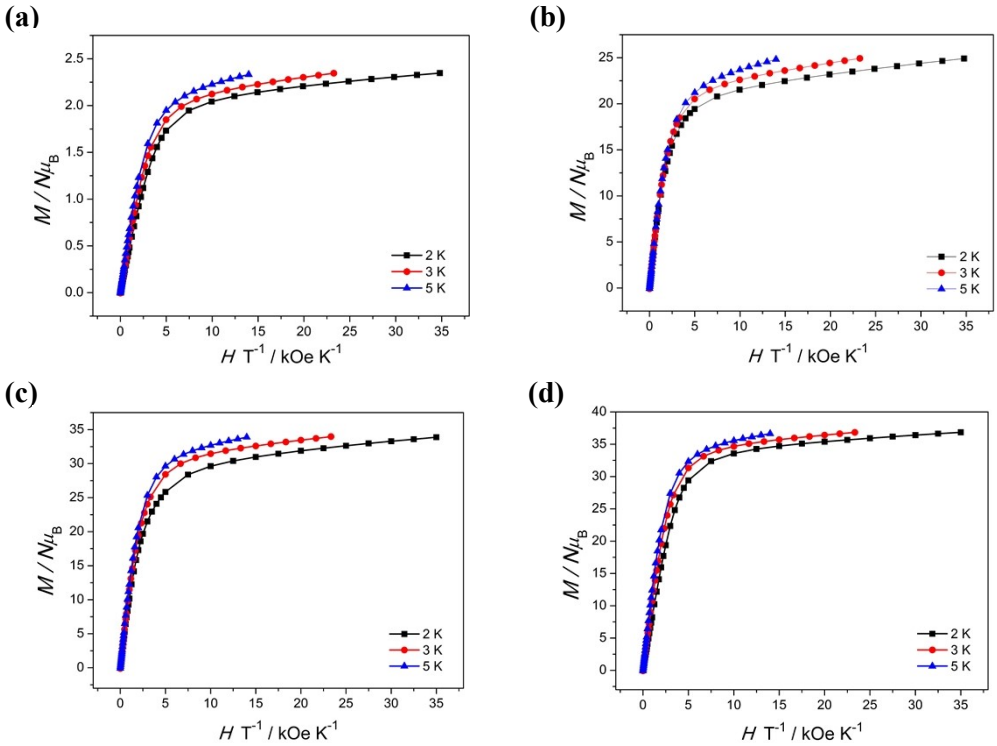

Fig. S17. M versus HT^{-1} plots under different temperatures for **Dy_2**(a); **Dy_4**(b)**;** **Dy_5**(c) and **Dy_6**(d).

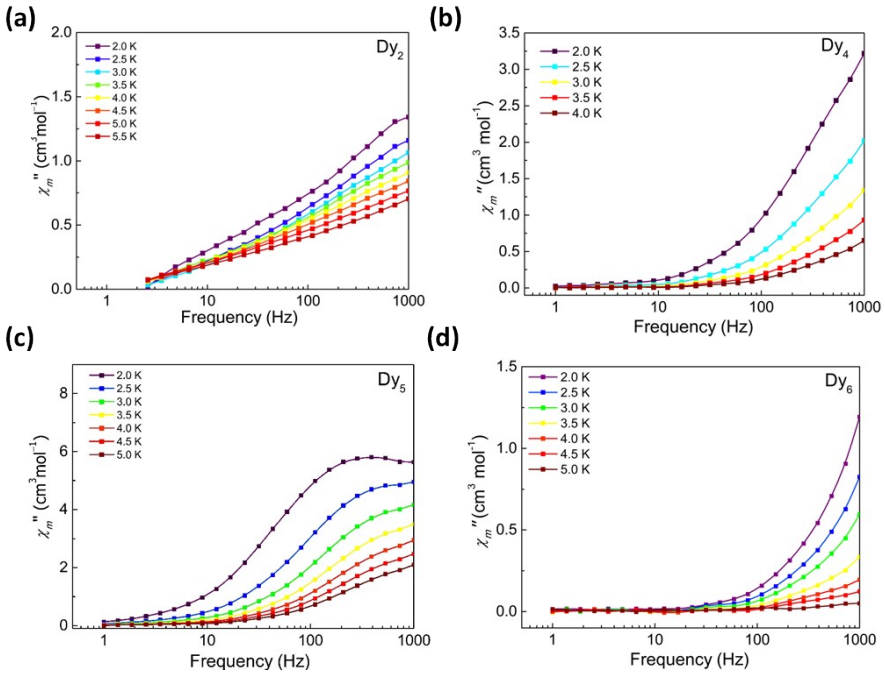

Fig.S18. Frequency dependence of the out-of-phase parts of the ac magnetic susceptibilities for **Dy_2-Dy_6** collected under a 0 Oe dc field at different temperature.

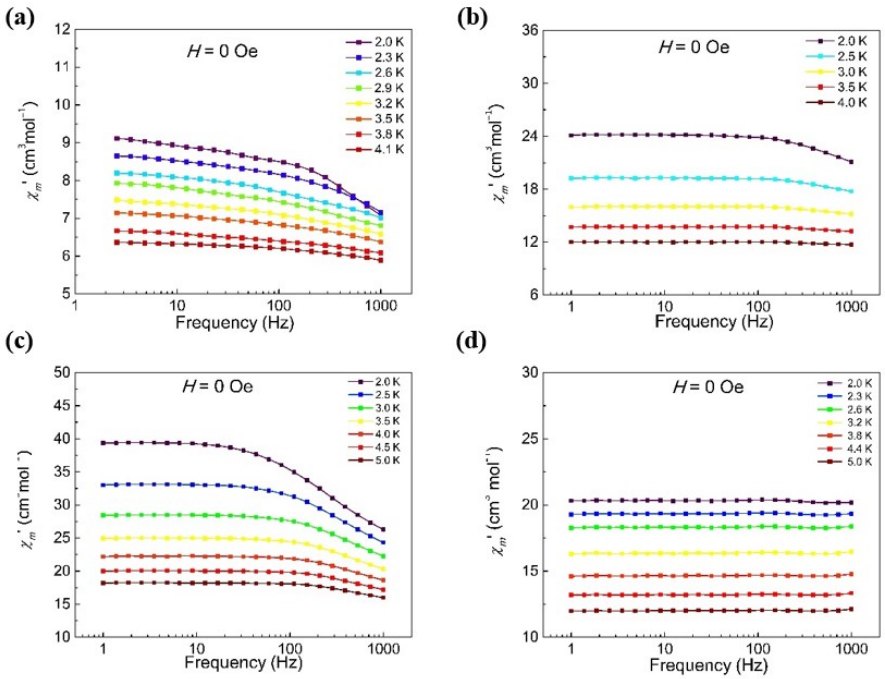

Fig. S19. Frequency-dependent in-phase (χ') ac susceptibilities under different dc fields for **Dy_2**(a); **Dy_4**(b); **Dy_5**(c) and **Dy_6**(d).

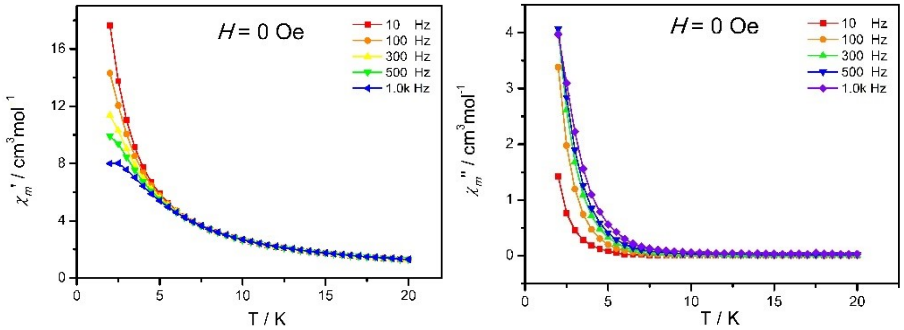

Fig. S20. Plots of in-phase ac susceptibilities (χ') and out-of-phase ac susceptibilities (χ") vs *T* at various frequencies under zero dc field for **Dy_2**.

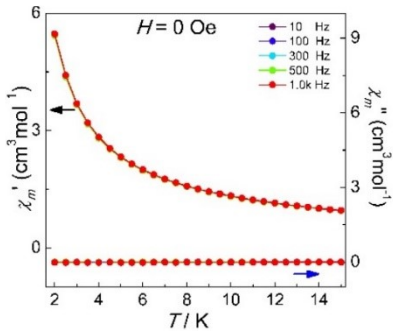

Fig. S21. Plots of in-phase ac susceptibilities (χ') and out-of-phase ac susceptibilities (χ") vs *T* at various frequencies under zero dc field for **Dy_4**.

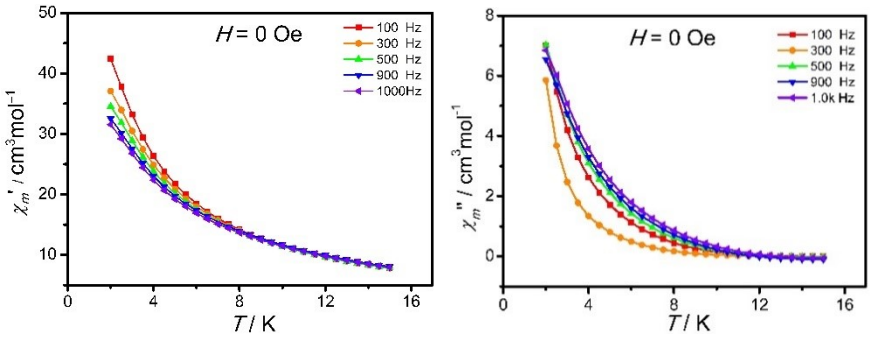

Fig. S22. Plots of in-phase ac susceptibilities (χ') and out-of-phase ac susceptibilities (χ") vs *T* at various frequencies under zero dc field for **Dy_5**.

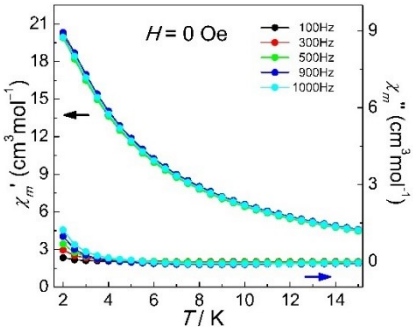

Fig. S23. Plots of in-phase ac susceptibilities (χ') and out-of-phase ac susceptibilities (χ") vs *T* at various frequencies under zero dc field for **Dy_6**.

Table S2. Detailed analysis results of the Contiouous Shape Measures (CShMs).

Lable	Dy1(**Dy_2**)	Dy1(**Dy_4**)	Dy2(**Dy_4**)	Dy2(**Dy_5**)	Dy1(**Dy_6**)	Dy2(**Dy_6**)	Dy3(**Dy_6**)
OP-8	29.23047	32.29623	31.30788	30.3577	29.65111	27.42542	30.48133
HPY-8	24.31967	22.51962	22.03174	23.69403	21.08121	21.89232	23.06941
HBPY-8	13.25771	15.06596	13.93922	16.45093	15.21084	16.96335	13.3407
CU-8	9.20705	10.77227	10.08064	11.65697	11.50213	10.33813	12.21268
SAPR-8	1.70037	3.0317	**1.61977**	3.23357	2.85824	**0.9402**	3.94187
TDD-8	2.41308	**1.15535**	3.51181	**0.58858**	2.13226	1.64063	**2.64899**
JGBF-8	10.31022	14.76593	13.46929	11.99969	13.14462	14.09724	11.36332
JETBPY-8	26.93511	27.36783	26.77363	28.17948	25.05975	26.18359	27.65307
JBTPR-8	**1.6368**	3.16298	3.18366	2.64982	2.61596	1.65911	3.74059
BTPR-8	1.65719	2.45899	2.50345	2.50636	**1.88203**	1.58007	3.06713
JSD-8	2.79538	4.09921	5.10584	1.70345	4.45543	3.26181	3.63779
TT-8	10.0414	11.1023	10.9095	12.1647	12.27688	10.85012	12.91911
ETBPY-8	22.29112	23.65115	21.2465	25.67421	21.36824	23.1605	22.32888
Lable	HP-87	HPY-7	PBPY-7	CO-7	CTPR-7	JPBPY-7	ETBPY-7
Dy1(**Dy_5**)	32.63884	21.88278	4.00485	1.88208	**1.09248**	6.78972	19.19307
Dy5(**Dy_5**)	33.3318	19.90714	6.82857	**0.36874**	1.1934	9.96678	19.15061

Table S3. Selected bond lengths / Å and bond angles / ° for **Dy_2**.

Bond Length/Å

Dy1—Dy2	3.792 (5)	Dy1—O13	2.349 (5)	Dy2—O9	2.503 (5)
Dy1—O4	2.398 (4)	Dy1—N6	2.522 (5)	Dy2—O10	2.405 (4)
Dy1—O3	2.509 (5)	Dy1—N4	2.528 (6)	Dy2—O14	2.361 (5)
Dy1—O10	2.300 (4)	Dy2—O2	2.264 (5)	Dy2—N1	2.536 (5)
Dy1—O8	2.269 (5)	Dy2—O4	2.306 (5)	Dy2—N3	2.510 (5)
Dy1—O12	2.264 (5)	Dy2—O6	2.245 (5)		

Bond Angles(°)

O4—Dy1—O3	65.74 (15)	O12—Dy1—O8	89.9 (2)	O4—Dy2—N3	71.37 (17)
O4—Dy1—N6	123.60 (17)	O12—Dy1—O13	149.23 (17)	O6—Dy2—O2	86.09 (19)
O4—Dy1—N4	137.67 (18)	O12—Dy1—N6	72.83 (18)	O6—Dy2—O4	109.75 (17)
O3—Dy1—N6	144.39 (18)	O12—Dy1—N4	138.06 (17)	O6—Dy2—O9	77.32 (18)
O3—Dy1—N4	130.67 (18)	O13—Dy1—O4	75.64 (16)	O6—Dy2—O10	78.45 (17)
O10—Dy1—O4	72.17 (15)	O13—Dy1—O3	77.60 (18)	O6—Dy2—O14	151.34 (18)
O10—Dy1—O3	135.92 (14)	O13—Dy1—N6	136.57 (19)	O6—Dy2—N1	135.25 (18)
O10—Dy1—O13	80.02 (17)	O13—Dy1—N4	72.40 (18)	O6—Dy2—N3	72.73 (18)
O10—Dy1—N6	72.04 (17)	N6—Dy1—N4	68.90 (19)	O9—Dy2—N1	130.32 (17)
O10—Dy1—N4	75.56 (19)	O2—Dy2—O4	150.36 (17)	O9—Dy2—N3	146.59 (18)
O8—Dy1—O4	139.32 (19)	O2—Dy2—O9	72.44 (17)	O10—Dy2—O9	65.33 (15)
O8—Dy1—O3	73.64 (18)	O2—Dy2—O10	137.20 (17)	O10—Dy2—N1	141.15 (17)
O8—Dy1—O10	147.4 (2)	O2—Dy2—O14	99.76 (18)	O10—Dy2—N3	121.08 (16)
O8—Dy1—O13	98.17 (18)	O2—Dy2—N1	74.16 (18)	O14—Dy2—O9	77.83 (18)
O8—Dy1—N6	88.81 (19)	O2—Dy2—N3	90.89 (19)	O14—Dy2—O10	78.38 (15)
O8—Dy1—N4	73.0 (2)	O4—Dy2—O9	134.30 (16)	O14—Dy2—N1	72.81 (17)
O12—Dy1—O4	78.91 (16)	O4—Dy2—O10	71.95 (15)	O14—Dy2—N3	134.59 (18)
O12—Dy1—O3	76.35 (17)	O4—Dy2—O14	78.50 (17)	N3—Dy2—N1	67.98 (17)
O12—Dy1—O10	108.28 (17)	O4—Dy2—N1	77.15 (17)	□	□

Table S4. Selected bond lengths / Å and bond angles / ° for **Dy_4**

Bond Length/Å

Dy1—Dy2	3.8533 (3)	Dy1—N1	2.484 (3)	Dy2—O7	2.312 (3)
Dy1—Dy2i	3.6063 (3)	Dy1—N3	2.600 (4)	Dy2—O7i	2.400 (2)
Dy1—Cl2	2.7548 (11)	Dy1—N2	2.550 (4)	Dy2—O2i	2.349 (3)
Dy1—Cl1	2.6536 (12)	Dy2—Dy2i	3.8600 (4)	Dy2—O6	2.316 (3)
Dy1—O7i	2.371 (3)	Dy2—Cl2i	2.8300 (12)	Dy2—O1i	2.454 (3)
Dy1—O2	2.350 (3)	Dy2—Cl3	2.6433 (13)	Dy2—O5	2.539 (3)
Dy1—O6	2.309 (3)				

Bond Angles(°)

Cl1—Dy1—Cl2	87.53 (4)	N1—Dy1—Cl2	100.07 (8)	$O7^{i}$—Dy2—O5	113.78 (9)
$O7^{i}$—Dy1—Cl2	74.02 (7)	N1—Dy1—Cl1	140.56 (9)	O7—Dy2—O5	80.43 (10)
$O7^{i}$—Dy1—Cl1	78.57 (7)	N1—Dy1—N3	68.29 (11)	$O2^{i}$—Dy2—$Cl2^{i}$	71.71 (7)
$O7^{i}$—Dy1—N1	140.80 (11)	N1—Dy1—N2	64.78 (11)	$O2^{i}$—Dy2—Cl3	113.50 (8)
$O7^{i}$—Dy1—N3	137.18 (10)	N3—Dy1—Cl2	143.08 (8)	$O2^{i}$—Dy2—$O7^{i}$	76.98 (9)
$O7^{i}$—Dy1—N2	143.38 (10)	N3—Dy1—Cl1	82.43 (8)	$O2^{i}$—Dy2—$O1^{i}$	66.08 (10)
O2—Dy1—Cl2	73.13 (7)	N2—Dy1—Cl2	75.57 (8)	$O2^{i}$—Dy2—O5	144.32 (10)
O2—Dy1—Cl1	146.84 (7)	N2—Dy1—Cl1	80.22 (9)	O6—Dy2—$Cl2^{i}$	143.48 (7)
O2—Dy1—$O7^{i}$	70.42 (9)	N2—Dy1—N3	67.75 (11)	O6—Dy2—Cl3	87.20 (8)

O2—Dy1—N1	70.82 (10)	Cl3—Dy2—Cl2^{i}	79.85 (4)	O6—Dy2—O7^{i}	68.85 (9)
O2—Dy1—N3	128.81 (10)	O7^{i}—Dy2—Cl2^{i}	137.63 (7)	O6—Dy2—O2^{i}	143.95 (9)
O2—Dy1—N2	118.83 (11)	O7—Dy2—Cl2^{i}	73.39 (7)	O6—Dy2—O1^{i}	92.39 (10)
O6—Dy1—Cl2	142.02 (7)	O7^{i}—Dy2—Cl3	140.01 (8)	O6—Dy2—O5	64.58 (10)
O6—Dy1—Cl1	95.09 (8)	O7—Dy2—Cl3	149.63 (7)	O1^{i}—Dy2—Cl2^{i}	117.23 (8)
O6—Dy1—O7^{i}	69.46 (9)	O7—Dy2—O7^{i}	70.00 (11)	O1^{i}—Dy2—Cl3	77.06 (7)
O6—Dy1—O2	85.01 (10)	O7—Dy2—O2^{i}	71.45 (9)	O1^{i}—Dy2—O5	148.80 (10)
O6—Dy1—N1	101.52 (10)	O7—Dy2—O6	105.88 (10)	O5—Dy2—Cl2^{i}	79.63 (8)
O6—Dy1—N3	74.50 (10)	O7^{i}—Dy2—O1^{i}	72.66 (9)	O5—Dy2—Cl3	80.87 (8)
O6—Dy1—N2	142.25 (11)	O7—Dy2—O1^{i}	128.19 (9)	□	□

Symmetry code: (i) -*x*+1, -*y*+1, -*z*.

Table S5. Selected bond lengths / Å and bond angles / ° for **Dy_5**

Bond Length/Å

Dy1—O4	2.270 (5)	Dy3—Dy1	3.6562 (6)	Dy4—O14	2.365 (6)
Dy1—O2	2.273 (6)	Dy3—O22	2.325 (6)	Dy4—O3	2.499 (5)
Dy1—O7	2.230 (5)	Dy3—O7	2.269 (5)	Dy4—O9	2.487 (5)
Dy1—O6	2.280 (6)	Dy3—O10	2.426 (5)	Dy4—O15	2.327 (6)
Dy1—O23	2.279 (6)	Dy3—O6	2.328 (5)	Dy4—Dy2	3.6228 (6)
Dy1—N1	2.407 (7)	Dy3—O12	2.328 (6)	Dy4—O8	2.418 (5)
Dy1—N3	2.496 (7)	Dy3—O13	2.387 (6)	Dy5—Dy3	3.7743 (6)
Dy1—Dy2	3.6440 (6)	Dy3—O5	2.582 (6)	Dy5—O10	2.323 (5)
Dy2—O2	2.431 (5)	Dy3—Dy2	3.7136 (6)	Dy5—O19	2.321 (6)
Dy2—O7	2.202 (5)	Dy3—O8	2.359 (5)	Dy5—O24^{i}	2.321 (5)
Dy2—O10	2.507 (6)	Dy4—Dy5	3.8409 (6)	Dy5—O17	2.386 (6)
Dy2—O16	2.348 (6)	Dy4—Dy3	3.5720 (6)	Dy5—O21	2.348 (6)
Dy2—O11	2.339 (6)	Dy4—Dy1	3.6463 (6)	Dy5—O9	2.284 (5)
Dy2—O9	2.435 (5)	Dy4—O4	2.403 (5)	Dy5—Dy2	3.8228 (6)
Dy2—O1	2.556 (6)	Dy4—O18	2.280 (5)	Dy5—O8	2.296 (5)
Dy2—O20	2.307 (6)	Dy4—O7	2.224 (5)		

Bond Angles(°)

O4—Dy1—O2	107.3 (2)	O9—Dy2—O1	134.80 (19)	O18—Dy4—O15	95.5 (2)
O4—Dy1—O6	93.8 (2)	O20—Dy2—O2	140.6 (2)	O18—Dy4—O8	77.78 (19)
O4—Dy1—O23	155.19 (19)	O20—Dy2—O10	78.4 (2)	O7—Dy4—O4	72.53 (18)
O4—Dy1—N1	80.3 (2)	O20—Dy2—O16	95.0 (2)	O7—Dy4—O18	144.12 (18)
O4—Dy1—N3	76.8 (2)	O20—Dy2—O11	93.9 (2)	O7—Dy4—O14	94.2 (2)
O2—Dy1—O6	134.1 (2)	O20—Dy2—O9	82.6 (2)	O7—Dy4—O3	137.10 (18)
O2—Dy1—O23	87.7 (2)	O20—Dy2—O1	76.8 (2)	O7—Dy4—O9	72.56 (18)
O2—Dy1—N1	76.7 (2)	O22—Dy3—O10	79.80 (19)	O7—Dy4—O15	93.8 (2)
O2—Dy1—N3	145.8 (2)	O22—Dy3—O6	140.82 (19)	O7—Dy4—O8	73.58 (19)
O7—Dy1—O4	75.05 (18)	O22—Dy3—O12	101.4 (2)	O14—Dy4—O4	73.84 (19)
O7—Dy1—O2	74.73 (19)	O22—Dy3—O13	84.8 (2)	O14—Dy4—O3	77.20 (19)
O7—Dy1—O6	72.00 (19)	O22—Dy3—O5	79.3 (2)	O14—Dy4—O9	140.49 (18)
O7—Dy1—O23	128.9 (2)	O22—Dy3—O8	82.45 (19)	O14—Dy4—O8	72.58 (18)
O7—Dy1—N1	134.2 (2)	O7—Dy3—O22	148.28 (19)	O9—Dy4—O3	137.19 (18)
O7—Dy1—N3	136.8 (2)	O7—Dy3—O10	72.54 (18)	O15—Dy4—O4	76.6 (2)
O6—Dy1—N1	148.4 (2)	O7—Dy3—O6	70.42 (18)	O15—Dy4—O14	145.3 (2)

O6—Dy1—N3	77.9 (2)	O7—Dy3—O12	87.1 (2)	O15—Dy4—O3	74.0 (2)
O23—Dy1—O6	89.3 (2)	O7—Dy3—O13	107.13 (19)	O15—Dy4—O9	73.90 (19)
O23—Dy1—N1	84.3 (2)	O7—Dy3—O5	131.88 (19)	O15—Dy4—O8	141.86 (19)
O23—Dy1—N3	79.8 (2)	O7—Dy3—O8	73.95 (18)	O8—Dy4—O3	138.52 (19)
N1—Dy1—N3	70.5 (2)	O10—Dy3—O5	135.91 (18)	O8—Dy4—O9	68.00 (17)
O2—Dy2—O10	132.89 (19)	O6—Dy3—O10	137.0 (2)	O10—Dy5—O17	147.32 (18)
O2—Dy2—O9	126.62 (19)	O6—Dy3—O12	80.7 (2)	O10—Dy5—O21	81.2 (2)
O2—Dy2—O1	63.78 (19)	O6—Dy3—O13	72.0 (2)	O19—Dy5—O10	77.7 (2)
O7—Dy2—O2	72.12 (19)	O6—Dy3—O5	64.46 (19)	O19—Dy5—O17	123.3 (2)
O7—Dy2—O10	72.06 (18)	O6—Dy3—O8	117.86 (18)	O19—Dy5—O21	115.2 (2)
O7—Dy2—O16	99.6 (2)	O12—Dy3—O10	76.4 (2)	O24^{i}—Dy5—O10	134.54 (19)
O7—Dy2—O11	91.9 (2)	O12—Dy3—O13	142.2 (2)	O24^{i}—Dy5—O19	74.7 (2)
O7—Dy2—O9	73.97 (18)	O12—Dy3—O5	70.3 (2)	O24^{i}—Dy5—O17	77.9 (2)
O7—Dy2—O1	135.90 (19)	O12—Dy3—O8	145.3 (2)	O24^{i}—Dy5—O21	78.9 (2)
O7—Dy2—O20	147.2 (2)	O13—Dy3—O10	141.0 (2)	O21—Dy5—O17	106.6 (2)
O10—Dy2—O1	141.41 (19)	O13—Dy3—O5	74.4 (2)	O9—Dy5—O10	75.22 (19)
O16—Dy2—O2	73.7 (2)	O8—Dy3—O10	70.33 (17)	O9—Dy5—O19	80.7 (2)
O16—Dy2—O10	142.04 (19)	O8—Dy3—O13	72.2 (2)	O9—Dy5—O24^{i}	133.10 (19)
O16—Dy2—O9	72.76 (19)	O8—Dy3—O5	143.1 (2)	O9—Dy5—O17	83.5 (2)
O16—Dy2—O1	69.5 (2)	O4—Dy4—O3	64.67 (18)	O9—Dy5—O21	147.99 (19)
O11—Dy2—O2	76.8 (2)	O4—Dy4—O9	131.92 (18)	O9—Dy5—O8	73.59 (18)
O11—Dy2—O10	74.9 (2)	O4—Dy4—O8	129.55 (18)	O8—Dy5—O10	73.27 (18)
O11—Dy2—O16	143.1 (2)	O18—Dy4—O4	143.35 (19)	O8—Dy5—O19	145.11 (19)
O11—Dy2—O9	144.0 (2)	O18—Dy4—O14	97.4 (2)	O8—Dy5—O24^{i}	140.16 (19)
O11—Dy2—O1	77.8 (2)	O18—Dy4—O3	78.71 (19)	O8—Dy5—O17	77.1 (2)
O9—Dy2—O10	69.34 (17)	O18—Dy4—O9	76.97 (19)	O8—Dy5—O21	79.16 (19)

Symmetry codes: (i) x+1/2, -y+3/2, z+1/2; (ii) x-1/2, -y+3/2, z-1/2.

Table S6. Selected bond lengths / Å and bond angles / ° for **Dy_6.**

Bond Length/Å					
Dy1—O2	2.279 (5)	Dy1—Dy2i	3.7825 (5)	Dy2—Dy2i	3.6276 (6)
Dy1—O6	2.282 (5)	Dy2—O8	2.305 (5)	Dy3—O10	2.280 (6)
Dy1—O8	2.323 (4)	Dy2—O9	2.322 (5)	Dy3—O16	2.285 (6)
Dy1—O15	2.342 (5)	Dy2—O8i	2.334 (4)	Dy3—O2	2.298 (5)
Dy1—O4	2.369 (5)	Dy2—O4i	2.359 (5)	Dy3—O7	2.348 (5)
Dy1—N3	2.466 (6)	Dy2—O7	2.375 (5)	Dy3—O13	2.429 (6)
Dy1—N1	2.483 (5)	Dy2—O6	2.41 (5)	Dy3—O12	2.440 (6)
Dy1—O7	2.526 (5)	Dy2—O3i	2.452 (5)	Dy3—O11	2.463 (6)
Dy1—Dy2	3.5181 (5)	Dy2—O5	2.499 (5)	Dy3—O14	2.509 (6)
Dy1—Dy3	3.7375 (5)				
Bond Angles(°)					
O2—Dy1—O6	135.28 (17)	O8—Dy2—O9	77.95 (17)	O10—Dy3—O16	155.9 (2)
O2—Dy1—O8	78.63 (16)	O8—Dy2—O8^{i}	77.12 (17)	O10—Dy3—O2	106.7 (2)
O6—Dy1—O8	69.78 (16)	O9—Dy2—O8^{i}	122.91 (18)	O16—Dy3—O2	88.8 (2)

O2—Dy1—O15	84.97 (18)	O8—Dy2—O4^{i}	117.20 (16)	O10—Dy3—O7	85.86 (19)
O6—Dy1—O15	106.3 (2)	O9—Dy2—O4^{i}	79.09 (17)	O16—Dy3—O7	80.70 (19)
O8—Dy1—O15	148.89 (18)	O8^{i}—Dy2—O4^{i}	68.53 (15)	O2—Dy3—O7	73.95 (17)
O2—Dy1—O4	114.31 (17)	O8—Dy2—O7	75.2 (16)	O10—Dy3—O13	76.1 (2)
O6—Dy1—O4	82.88 (17)	O9—Dy2—O7	80.04 (17)	O16—Dy3—O13	124.8 (2)
O8—Dy1—O4	68.53 (15)	O8^{i}—Dy2—O7	138.57 (16)	O2—Dy3—O13	84.4 (2)
O15—Dy1—O4	142.56 (18)	O4^{i}—Dy2—O7	152.63 (16)	O7—Dy3—O13	146.5 (2)
O2—Dy1—N3	143.91 (18)	O8—Dy2—O6	68.05 (16)	O10—Dy3—O12	86.0 (2)
O6—Dy1—N3	79.08 (18)	O9—Dy2—O6	139.37 (18)	O16—Dy3—O12	88.8 (2)
O8—Dy1—N3	133.56 (17)	O8^{i}—Dy2—O6	70.99 (16)	O2—Dy3—O12	151.7 (2)
O15—Dy1—N3	72.15 (19)	O4^{i}—Dy2—O6	136.10 (16)	O7—Dy3—O12	133.3 (2)
O4—Dy1—N3	74.28 (18)	O7—Dy2—O6	70.42 (16)	O13—Dy3—O12	74.0 (2)
O2—Dy1—N1	77.48 (18)	O8—Dy2—O3^{i}	151.25 (17)	O10—Dy3—O11	79.8 (2)
O6—Dy1—N1	146.48 (18)	O9—Dy2—O3^{i}	74.53 (19)	O16—Dy3—O11	78.4 (2)
O8—Dy1—N1	121.67 (19)	O8^{i}—Dy2—O3^{i}	125.48 (17)	O2—Dy3—O11	153.9 (2)
O15—Dy1—N1	79.3 (2)	O4^{i}—Dy2—O3^{i}	65.38 (16)	O7—Dy3—O11	81.5 (2)
O4—Dy1—N1	74.54 (18)	O7—Dy2—O3^{i}	92.06 (17)	O13—Dy3—O11	121.5 (2)
N3—Dy1—N1	71.2 (2)	O6—Dy2—O3^{i}	132.15 (17)	O12—Dy3—O11	51.8 (2)
O2—Dy1—O7	70.90 (16)	O8—Dy2—O5	132.73 (16)	O10—Dy3—O14	126.7 (2)
O6—Dy1—O7	69.66 (16)	O9—Dy2—O5	145.40 (18)	O16—Dy3—O14	73.9 (2)
O8—Dy1—O7	71.86 (16)	O8^{i}—Dy2—O5	84.77 (17)	O2—Dy03—O14	78.0 (2)
O15—Dy1—O7	77.87 (18)	O4^{i}—Dy2—O5	95.05 (18)	O7—Dy3—O14	142.21 (19)
O4—Dy1—O7	137.60 (15)	O7—Dy2—O5	92.16 (18)	O13—Dy3—O14	51.1 (2)
N3—Dy1—O7	127.85 (18)	O6—D2—O5	64.80 (17)	O12—Dy3—O14	74.2 (2)
N1—Dy1—O7	142.24 (17)	O3^{i}—Dy2—O5	72.12 (18)	O11—Dy3—O14	119.0 (2)

Symmetry code: (i) -x+1, -y+1, -z+1.