

# Mononuclear Dysprosium(III) complexes with triphenylphosphine oxide ligands: controlling the coordination environment and magnetic anisotropy

Stuart K. Langley<sup>1\*</sup>, Kuduva R. Vignesh<sup>2</sup>, Kerey Holton<sup>1</sup>, Sophie Benjamin<sup>3</sup>, Gary Hix<sup>4</sup>, Wasinee Phonsri<sup>5</sup>, Boujemaa Moubaraki<sup>5</sup>, Keith S. Murray<sup>5\*</sup> and Gopalan Rajaraman<sup>2\*</sup>

**Table S1.** Shape measures of the 9- and 8-coordinate of Dy coordination polyhedra in **1** and **2**, respectively.

Polyhedron <sup>a</sup>	Complex 1	Polyhedron <sup>b</sup>	Complex 2
EP-9	33.80	OP-8	28.63
OPY-9	23.01	HPY-8	24.38
HBPY-9	17.60	HBPY-8	12.93
JTC-9	14.29	CU-8	11.85
JCCU-9	10.63	SAPR-8	4.94
CCU-9	9.56	TDD-8	<b>2.49</b>
JCSAPR-9	2.69	JGBF-8	9.55
CSAPR-9	<b>1.94</b>	JETBPY-8	24.94
JTCTPR-9	3.37	JBTPR-8	3.90
HH-9	9.78	BTPR-8	3.67
MFF-9	1.93	JSD-8	2.45
		TT-8	12.68
		ETBPY-8	22.56

<sup>a</sup>Abbreviations: EP-9 Enneagon; OPY-9 Octagonal pyramid; HBPY-9 Heptagonal bipyramid; JTC-9 Triangular cupola = trivacant cuboctahedron; JCCU-9 Capped cube (Elongated square pyramid); CCU-9 Capped cube; JCSAPR-9 Capped sq. antiprism (Gyroelongated square pyramid) ; CSAPR-9 Capped square antiprism; JTCTPR-9 Tricapped trigonal prism; TCTPR-9 Tricapped trigonal prism; JTDIC-9 Tridiminished icosahedron; HH-9 Hula-hoop; MFF-9 Muffin

<sup>b</sup>Abbreviations: OP-8, octagon; HPY-8, heptagonal pyramid; HBPY-8, hexagonal bipyramid; CU-8, cube; SAPR-8, square antiprism; TDD-8, triangular dodecahedron; JGBF-8, Johnson gyrobifastigium; JETBPY-8, Johnson elongated triangular bipyramid; JBTPR-8, Johnson biaugmented trigonal prism; BTPR-8, biaugmented trigonal prism; JSD-8, Johnson snub diphendoid; TT-8, triakis tetrahedron; ETBPY-8, elongated trigonal bipyramid.

**Table S2.** Shape measures of the 6-coordinate Dy coordination polyhedra in **3-5**.

Polyhedron <sup>c</sup>	Complex 3	Complex 4	Complex 5
HP-6	33.46	33.05	33.12
PPY-6	27.81	28.86	29.19
OC-6	<b>0.63</b>	<b>0.60</b>	<b>0.59</b>
TPR-6	15.11	16.24	16.56
JPPY-6	31.34	31.94	32.28
<sup>c</sup> Abbreviations: HP-6 Hexagon; PPY-6 Pentagonal pyramid; OC-6 Octahedron; TPR-6 Trigonal prism ; JPPY-5 Johnson pentagonal pyramid.			

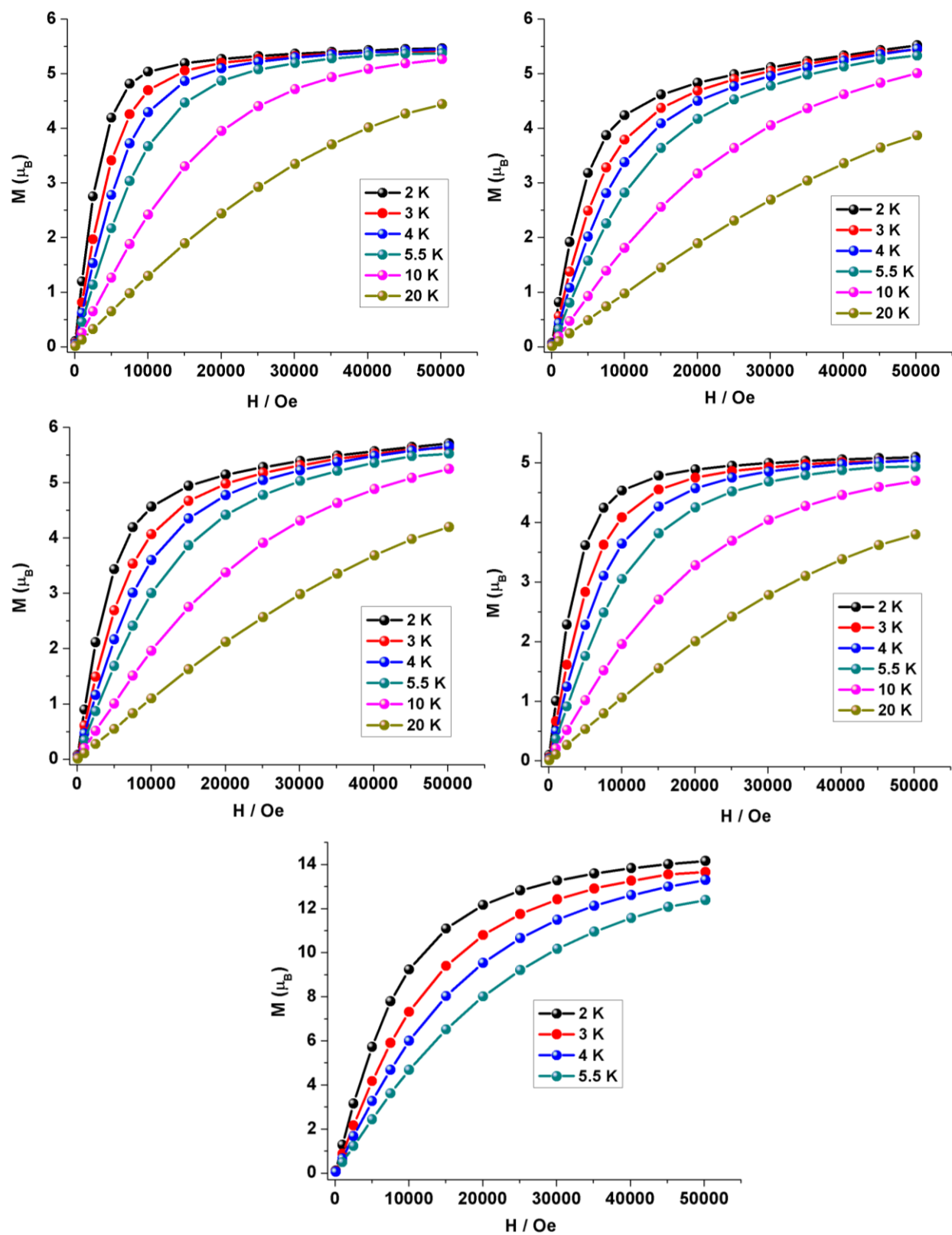
**Table S3.** Bond length data (Å) for **1 – 5**.

<b>1</b>		<b>2</b>		<b>3</b>		<b>3'</b>	
Dy-O3	2.2778(14)	Dy-O5'	2.247(4)	Dy1-O1	2.2249(18)	Dy2-O6	2.2436(18)
Dy-O2	2.2830(15)	Dy-O5	2.247(4)	Dy1-O3	2.2351(18)	Dy2-O5	2.2577(17)
Dy-O1	2.2951(14)	Dy-O6'	2.284(4)	Dy1-O2	2.2876(18)	Dy2-O4	2.2617(18)
Dy-O10	2.4388(15)	Dy-O6	2.284(4)	Dy1-Cl2	2.6139(7)	Dy2-Cl5	2.5991(8)
Dy-O4	2.4537(17)	Dy-O1'	2.451(4)	Dy1-Cl1	2.6328(10)	Dy2-Cl4	2.6297(18)
Dy-O7	2.4631(17)	Dy-O1	2.451(4)	Dy1-Cl3	2.6342(10)	Dy2-Cl6	2.6470(9)
Dy-O5	2.4814(17)	Dy-O2'	2.481(4)				
Dy-O8	2.4877(17)	Dy-O2	2.481(4)				
Dy-O11	2.5127(16)						

<b>4</b>		<b>4'</b>		<b>4''</b>	
Dy1-O9'	2.231(4)	Dy2-O4	2.231(4)	Dy3-O13	2.216(5)
Dy1-O9	2.231(4)	Dy2-O6	2.245(4)	Dy3-O17	2.228(5)
Dy1-O11'	2.246(4)	Dy2-O5	2.251(4)	Dy3-O8	2.233(6)
Dy1-O11	2.246(4)	Dy2-O7	2.251(4)	Dy3-O15	2.265(7)
Dy1-Cl8	2.601(2)	Dy2-Cl7	2.6194(15)	Dy3-Cl9	2.6164(16)
Dy1-Cl11	2.620(2)	Dy2-Cl14	2.62221(15)	Dy3-Cl19	2.6444(19)

<b>5</b>		<b>5'</b>	
Dy1-O11	2.2245(19)	Dy2-O8	2.231(2)
Dy1-O5	2.230(2)	Dy2-O10	2.243(2)
Dy1-O9	2.2424(19)	Dy2-O6	2.244(2)
Dy1-O7	2.244(2)	Dy2-O12	2.2519(19)
Dy1-Cl5	2.6138(7)	Dy2-Cl6	2.6170(7)
Dy1-Cl3	2.6302(7)	Dy2-Cl4	2.6258(7)

Complex **3**, **4** and **5** have two, three and two unique metal ions in the asymmetric unit, respectively.



**Figure S1.** Plots of  $M$  versus  $H$  isotherms for complexes 1 (top left), 2 (top right), 3 (middle left), 4 (middle right) and 5 (bottom) at 2, 3, 4, 5.5, 10 and 20 K.

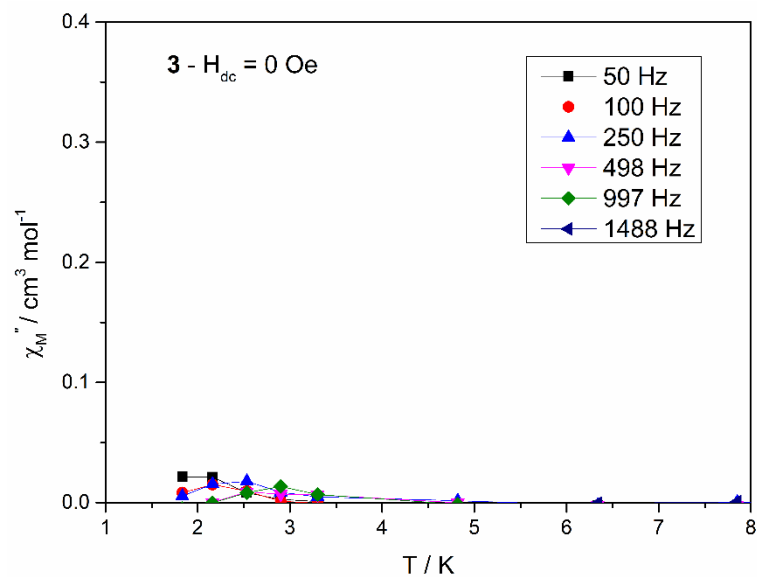


Figure S2. Plot of  $\chi''$  versus  $T$  for complex 3 ( $H_{dc} = 0$  Oe).

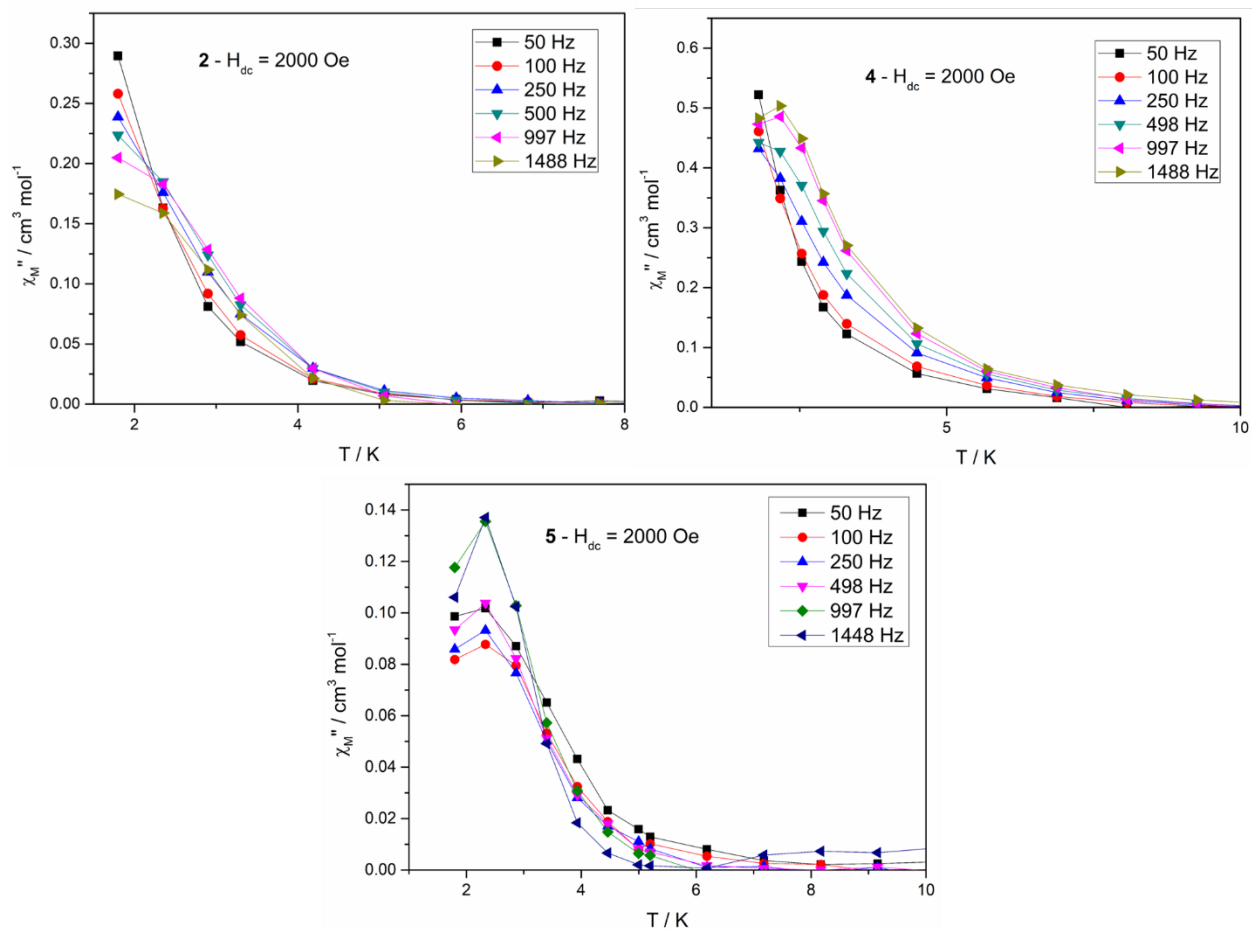
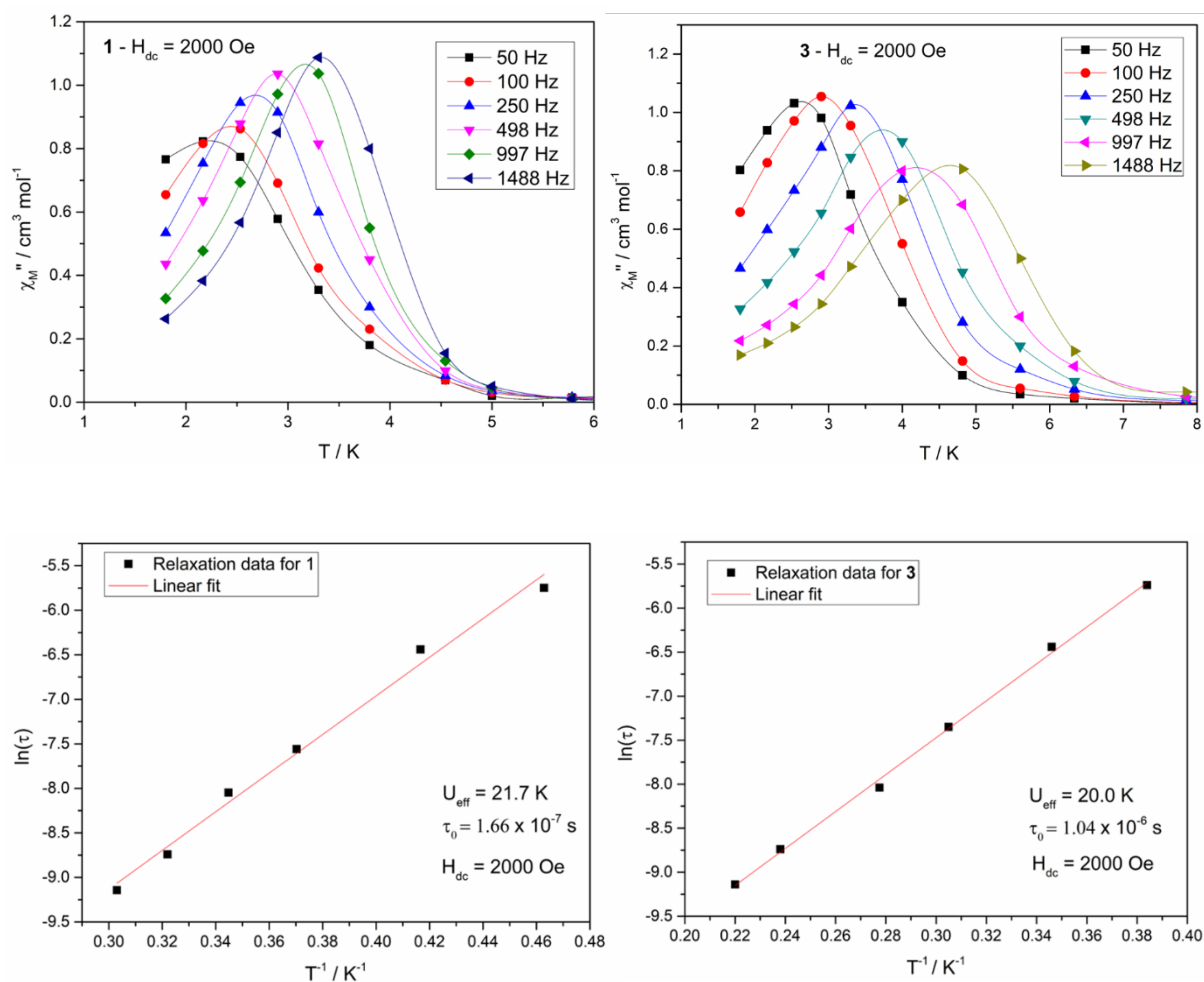


Figure S3. Plots of  $\chi''$  versus  $T$  for complexes 2 (top left), 4 (top right) and 5 (bottom) ( $H_{dc} = 2000$  Oe).



**Figure S4.**  $\chi_M''$  vs  $T$  for **1** (top left) and **3** (top right),  $H_{dc} = 2000 \text{ Oe}$  and  $\ln(\tau)$  vs  $T^{-1}$  plots for **1** (bottom left) and **3** (bottom right) and **3**.

**Table S4.** The  $g$ -tensor for the eight lowest Kramer's doublets in 1–5.

KDs		1	2	3	4	5
1	$g_x$	0.2287	11.9707	0.1352	2.1939	1.2982
	$g_y$	0.3597	8.0477	2.9545	5.9830	2.8906
	$g_z$	19.6158	0.7205	16.6803	11.6635	15.6449
2	$g_x$	1.2424	11.2464	1.8559	11.5699	2.2349
	$g_y$	2.5797	7.5039	3.3976	6.5171	4.2730
	$g_z$	14.5400	0.9077	13.9374	1.1546	12.8135
3	$g_x$	1.3167	1.7696	0.9956	1.1166	1.4306
	$g_y$	1.7468	2.8407	1.8251	1.7863	5.4318
	$g_z$	14.7510	9.4798	15.6905	15.3274	11.4788
4	$g_x$	2.4863	2.2134	6.3739	8.3977	8.5502
	$g_y$	4.8001	2.4132	6.5877	7.8569	7.7033
	$g_z$	11.7698	9.5985	9.3806	6.2360	6.2214
5	$g_x$	2.9324	0.4623	0.3279	4.2247	4.6444
	$g_y$	4.8141	1.53721	1.8457	5.0178	4.7493
	$g_z$	10.5919	5.6883	9.7869	9.7629	8.9256
6	$g_x$	0.0307	0.5387	3.3439	0.6628	0.7248
	$g_y$	0.5252	3.0373	5.7538	4.0157	4.8613
	$g_z$	16.8932	12.4774	8.5144	10.1471	9.7919
7	$g_x$	1.2355	5.7461	1.2156	1.1354	1.5209
	$g_y$	2.4115	4.3488	4.8003	4.7161	5.4493
	$g_z$	14.5844	2.2037	11.0804	10.4895	10.6602
8	$g_x$	0.6562	1.9784	3.0217	1.0700	12.1916
	$g_y$	0.8414	6.0334	4.0270	4.8155	6.2188
	$g_z$	17.9767	13.7132	13.0809	14.3456	0.2044

**Table S5.** RASSI energies of the lowest spin-orbit states (cm<sup>-1</sup>) of each Dy center in complexes **1–5**.

1	2	3	4	5
0.000	0.000	0.000	0.000	0.000
48.293	7.044	30.526	31.509	31.637
88.199	125.787	64.225	53.241	52.888
148.413	148.122	145.911	148.318	153.478
184.968	185.368	276.868	294.835	302.001
212.832	231.406	307.394	322.282	331.027
265.940	274.568	343.395	364.666	374.866
333.096	312.126	367.989	394.842	396.745
2998.457	3042.847	3080.513	3096.466	3096.548
3078.931	3060.782	3112.342	3104.176	3119.985
3111.834	3127.015	3132.055	3134.481	3134.512
3140.086	3139.493	3177.059	3191.327	3194.629
3160.756	3155.275	3194.545	3202.727	3211.924
3193.845	3189.750	3206.441	3216.517	3221.424
3235.516	3202.365	3228.202	3245.340	3248.996
5599.010	5630.039	5691.628	5696.105	5702.701
5649.963	5669.236	5709.323	5715.211	5722.561
5691.919	5686.501	5723.030	5738.878	5741.366
5703.541	5716.469	5737.866	5744.456	5748.919
5767.678	5740.660	5756.134	5763.637	5769.227
5810.452	5777.521	5774.769	5785.472	5789.729
7796.391	7801.743	7859.772	7863.653	7868.423
7825.211	7850.964	7879.909	7884.833	7892.419
7864.307	7877.787	7893.881	7906.504	7907.355
7929.509	7917.383	7907.619	7911.213	7917.334
7981.340	7946.275	7983.165	7997.945	8003.166
9513.605	9539.161	9552.260	9558.796	9563.490
9554.117	9552.849	9559.642	9563.966	9568.029
9573.391	9559.864	9590.834	9598.367	9603.230
9579.636	9571.703	9628.687	9634.759	9638.898
9594.790	9602.521	9638.516	9647.948	9652.464
9620.655	9618.208	9663.221	9670.989	9675.726
9652.960	9660.936	9675.302	9686.175	9691.547
9672.843	9688.985	9684.070	9698.200	9703.282
9708.340	9704.855	9702.453	9715.652	9722.278
9772.469	9725.864	9807.798	9832.574	9839.002
10952.922	10987.386	11015.531	11025.463	11030.321
11058.322	11027.511	11043.610	11043.072	11048.097
11134.713	11136.014	11169.879	11187.167	11191.814
11733.862	11733.892	11771.363	11782.533	11787.738
11768.627	11763.598	11782.312	11794.467	11799.370
11788.934	11772.959	11814.185	11827.755	11832.846
11794.146	11803.706	11825.932	11840.309	11846.341
11816.730	11819.779	11863.263	11881.048	11886.820
13517.738	13496.855	13496.664	13503.401	13507.331

13548.786	13543.498	13601.424	13614.623	13620.234
13565.978	13590.596	13609.008	13624.123	13629.136
13603.310	13599.997	13641.980	13658.848	13664.892
14919.702	14903.911	14914.801	14923.320	14927.600
14946.750	14950.046	14993.825	15008.197	15013.455
14963.838	14971.180	14997.168	15011.388	15016.736
15929.484	15929.147	15962.926	15976.192	15981.560
15938.919	15939.403	15965.609	15979.339	15984.195
16528.153	16526.815	16553.742	16566.604	16571.520
38806.558	38830.069	38872.599	38886.622	38894.574
38861.964	38870.608	38883.636	38898.783	38904.141
38905.342	38900.112	38896.196	38911.604	38914.102
38975.890	38943.149	38916.839	38932.691	38930.355
40189.730	40212.308	40250.213	40264.565	40273.590
40278.703	40271.834	40280.548	40295.422	40297.743
40387.794	40346.315	40301.217	40317.445	40314.845
41261.416	41255.955	41261.420	41276.434	41280.295
41298.538	41281.167	41271.330	41286.657	41288.251



**Table S6.** SINGLE\_ANISO computed crystal field parameters for complexes **1** – **5**. The major components in the Table are in bold.  $B_k^q$  is the crystal field parameter and  $O_k^q$  is the extended Stevens operator. The quantization axis is chosen to be the main magnetic axis of the ground pseudo-Doublet. See Equation 2.

k	q	$B_k^q$	$B_k^q$	$B_k^q$	$B_k^q$	$B_k^q$
		<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>
2	-2	<b>-0.74</b>	0.001	0.03	-0.11	0.05
	-1	0.05	<b>0.85</b>	<b>-0.52</b>	<b>0.72</b>	<b>-0.36</b>
	0	<b>-1.19</b>	0.11	-0.27	-0.23	-0.21
	1	0.24	-0.002	0.19	0.14	<b>0.34</b>
	2	<b>1.04</b>	<b>-0.72</b>	0.27	0.21	-0.05
4	-4	0.01	-0.0001	-0.004	-0.001	0.001
	-3	-0.005	-0.03	0.01	-0.05	0.01
	-2	0.008	-0.0002	0.001	0.001	0.0001
	-1	0.005	0.006	0.01	-0.05	0.01
	0	-0.003	-0.002	-0.01	-0.01	-0.01
	1	0.005	-0.0001	-0.001	-0.0001	-0.004
	2	-0.001	0.002	0.002	0.009	0.005
	3	0.01	-0.0001	-0.002	0.007	0.004
	4	-0.01	0.05	-0.04	-0.05	-0.05
	6	$2.49 \times 10^{-4}$	$-4.62 \times 10^{-7}$	$1.75 \times 10^{-5}$	$1.28 \times 10^{-5}$	$-6.87 \times 10^{-6}$
6	-5	$1.25 \times 10^{-4}$	$-1.27 \times 10^{-4}$	$1.92 \times 10^{-4}$	$-6.72 \times 10^{-4}$	$1.56 \times 10^{-4}$
	-4	$-1.44 \times 10^{-5}$	$6.42 \times 10^{-7}$	$-2.97 \times 10^{-5}$	$-3.33 \times 10^{-5}$	$9.42 \times 10^{-6}$
	-3	$-1.0 \times 10^{-4}$	$-1.18 \times 10^{-4}$	$1.23 \times 10^{-4}$	$-3.75 \times 10^{-4}$	$8.95 \times 10^{-5}$
	-2	$-2.66 \times 10^{-5}$	$-9.72 \times 10^{-7}$	$-3.39 \times 10^{-6}$	$1.18 \times 10^{-5}$	$-5.38 \times 10^{-6}$
	-1	$-8.45 \times 10^{-5}$	$2.68 \times 10^{-4}$	$-6.14 \times 10^{-5}$	$1.46 \times 10^{-4}$	$-3.39 \times 10^{-5}$
	0	$2.54 \times 10^{-5}$	$-1.64 \times 10^{-5}$	$2.18 \times 10^{-5}$	$1.24 \times 10^{-5}$	$2.11 \times 10^{-5}$
	1	$-8.69 \times 10^{-5}$	$6.58 \times 10^{-7}$	$2.22 \times 10^{-6}$	$-3.81 \times 10^{-6}$	$1.11 \times 10^{-5}$
	2	$3.20 \times 10^{-5}$	$4.37 \times 10^{-5}$	$1.31 \times 10^{-5}$	$9.04 \times 10^{-6}$	$3.51 \times 10^{-5}$
	3	$1.01 \times 10^{-4}$	$4.01 \times 10^{-6}$	$-1.11 \times 10^{-5}$	$5.81 \times 10^{-5}$	$4.00 \times 10^{-5}$
	4	$2.04 \times 10^{-4}$	$4.13 \times 10^{-5}$	$-2.37 \times 10^{-4}$	$-1.75 \times 10^{-4}$	$-2.95 \times 10^{-4}$
	5	$1.08 \times 10^{-4}$	$7.31 \times 10^{-6}$	$-4.01 \times 10^{-6}$	$1.23 \times 10^{-4}$	$-5.98 \times 10^{-5}$
	6	$-1.50 \times 10^{-4}$	$-5.94 \times 10^{-5}$	$3.43 \times 10^{-5}$	$-1.88 \times 10^{-5}$	$7.70 \times 10^{-5}$

**Table S7.** Experimental X-ray data.

	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>
Formula <sup>A</sup>	DyC <sub>60</sub> H <sub>57</sub> O <sub>14</sub> N <sub>3</sub> P <sub>3</sub>	DyC <sub>72</sub> H <sub>60</sub> O <sub>13</sub> N <sub>3</sub> P <sub>4</sub>	DyC <sub>55.5</sub> H <sub>48</sub> O <sub>3.50</sub> Cl <sub>3</sub> P <sub>3</sub>	DyC <sub>72</sub> H <sub>60</sub> O <sub>4</sub> Cl <sub>3</sub> P <sub>4</sub>	DyC <sub>42</sub> H <sub>60</sub> O <sub>24</sub> N <sub>4</sub>
M, g mol <sup>-1</sup>	1299.50	1454.00	1132.70	1381.93	1544.13
Crystal system	monoclinic	Orthorhombic	Monoclinic	Monoclinic	Triclinic
Space group	<i>P2<sub>1</sub>/n</i>	<i>Pccn</i>	<i>P2<sub>1</sub>/c</i>	<i>C2/c</i>	<i>P-1</i>
a/[Å]	11.040(2)	16.0038(8)	19.684(4)	35.8608(10)	19.4549(2)
b/[Å]	19.136(4)	16.5124(4)	15.211(3)	43.6134(13)	19.8966(3)
c/[Å]	27.568(6)	26.6249(10)	34.082(7)	26.6974(7)	19.9214(3)
α/[°]	90	90	90	90	90.3010(10)
β/[°]	94.95(3)	90	95.91(3)	96.885(3)	96.2960(10)
γ/[°]	90	90	90	90	115.6120(10)
V/[Å <sup>3</sup> ]	5802(2)	7035.9(6)	2622.9(17)	41454(2)	6899.72(16)
T/K	123(2)	123(2)	123(2)	123(2)	123(2)
Z	4	4	8	20	4
ρ <sub>calc</sub> [g cm <sup>-3</sup> ]	1.488	1.380	1.482	1.107	1.486
Δ <sup>B</sup> /[Å]	0.71073	0.71073	0.71073	0.71073	0.71073
Data Measured	94316	68643	167503	100982	149199
Ind. Reflns	13724	8081	24163	40661	31378
R <sub>int</sub>	0.0290	0.0679	0.0490	0.0538	0.0475
Reflns with I > 2σ(I)	13141	6095	23070	27425	26632
Parameters	734	457	1227	1915	1585
Restraints	0	38	0	0	0
R <sub>1</sub> <sup>C</sup> (obs), wR <sub>2</sub> <sup>C</sup> (all)	0.0312, 0.0833	0.0637, 0.1853	0.0322, 0.0826	0.0640, 0.1776	0.0377, 0.0745
goodness of fit	1.047	1.124	1.076	1.022	1.064
Largest residuals/[e Å <sup>-3</sup> ]	0.808, -1.486	2.159, -1.049	1.720, -1.560	5.513, -6.606	2.012, -1.264

**Table S8.** Ab initio computed magnetic susceptibility ( $\chi T$ ) vs. Temperature (T) data for complexes **1** – **5**.

Complex <b>1</b>		Complex <b>2</b>		Complex <b>3</b>		Complex <b>4</b>		Complex <b>5</b>	
T	$\chi T$	T	$\chi T$	T	$\chi T$	T	$\chi T$	T	$\chi T$
1E-4	12.03473	1E-4	6.52085	1E-4	8.97161	1E-4	5.52242	1E-4	12.33576
3.0303	12.20402	3.0303	9.88178	3.0303	9.49832	3.0303	6.78696	3.0303	12.93715
6.06061	12.37327	6.06061	11.40351	6.06061	10.02242	6.06061	8.02715	6.06061	13.53705
9.09091	12.54029	9.09091	11.93654	9.09091	10.51744	9.09091	9.11559	9.09091	14.11824
12.12121	12.69641	12.12121	12.18309	12.12121	10.94784	12.12121	9.9702	12.12121	14.6503
15.15152	12.83288	15.15152	12.33164	15.15152	11.30407	15.15152	10.61262	15.15152	15.1129
18.18182	12.94706	18.18182	12.43983	18.18182	11.59395	18.18182	11.09348	18.18182	15.50093
21.21212	13.04097	21.21212	12.52876	21.21212	11.83001	21.21212	11.45788	21.21212	15.82009
24.24242	13.11835	24.24242	12.60721	24.24242	12.02404	24.24242	11.73937	24.24242	16.08104
27.27273	13.18297	27.27273	12.67914	27.27273	12.18563	27.27273	11.9616	27.27273	16.2951
30.30303	13.23802	30.30303	12.74644	30.30303	12.32216	30.30303	12.14093	30.30303	16.47229
33.33333	13.28595	33.33333	12.81006	33.33333	12.43915	33.33333	12.2887	33.33333	16.62073
36.36364	13.32856	36.36364	12.87048	36.36364	12.54071	36.36364	12.41277	36.36364	16.7467
39.39394	13.36713	39.39394	12.928	39.39394	12.62992	39.39394	12.51874	39.39394	16.85498
42.42424	13.40256	42.42424	12.9828	42.42424	12.7091	42.42424	12.61059	42.42424	16.94919
45.45455	13.43548	45.45455	13.03502	45.45455	12.78005	45.45455	12.69125	45.45455	17.03208
48.48485	13.46634	48.48485	13.08478	48.48485	12.84414	48.48485	12.7629	48.48485	17.10575
51.51515	13.49543	51.51515	13.13218	51.51515	12.90247	51.51515	12.82717	51.51515	17.17184
54.54545	13.52298	54.54545	13.17733	54.54545	12.95592	54.54545	12.88533	54.54545	17.23161
57.57576	13.54915	57.57576	13.22032	57.57576	13.00519	57.57576	12.93838	57.57576	17.28608
60.60606	13.57406	60.60606	13.26125	60.60606	13.05085	60.60606	12.9871	60.60606	17.33605
63.63636	13.59779	63.63636	13.30021	63.63636	13.09336	63.63636	13.03211	63.63636	17.38216
66.66667	13.62044	66.66667	13.3373	66.66667	13.13312	66.66667	13.07392	66.66667	17.42495
69.69697	13.64204	69.69697	13.37259	69.69697	13.17045	69.69697	13.11295	69.69697	17.46484
72.72727	13.66267	72.72727	13.40618	72.72727	13.20562	72.72727	13.14955	72.72727	17.5022
75.75758	13.68236	75.75758	13.43813	75.75758	13.23884	75.75758	13.18398	75.75758	17.53731
78.78788	13.70115	78.78788	13.46853	78.78788	13.27032	78.78788	13.21649	78.78788	17.57043
81.81818	13.7191	81.81818	13.49746	81.81818	13.30022	81.81818	13.24728	81.81818	17.60177
84.84848	13.73623	84.84848	13.52497	84.84848	13.32867	84.84848	13.27652	84.84848	17.63151
87.87879	13.75258	87.87879	13.55115	87.87879	13.35579	87.87879	13.30435	87.87879	17.65979
90.90909	13.76819	90.90909	13.57605	90.90909	13.38169	90.90909	13.33089	90.90909	17.68674
93.93939	13.78309	93.93939	13.59974	93.93939	13.40645	93.93939	13.35625	93.93939	17.71248
96.9697	13.79732	96.9697	13.62228	96.9697	13.43015	96.9697	13.38052	96.9697	17.73709
100	13.8109	100	13.64373	100	13.45286	100	13.40377	100	17.76067
103.0303	13.82387	103.0303	13.66415	103.0303	13.47465	103.0303	13.42608	103.0303	17.78329
106.06061	13.83626	106.06061	13.68358	106.06061	13.49557	106.06061	13.44752	106.06061	17.805
109.09091	13.84808	109.09091	13.70208	109.09091	13.51566	109.09091	13.46812	109.09091	17.82588
112.12121	13.85939	112.12121	13.7197	112.12121	13.53497	112.12121	13.48794	112.12121	17.84595
115.15152	13.87018	115.15152	13.73648	115.15152	13.55354	115.15152	13.50703	115.15152	17.86529
118.18182	13.8805	118.18182	13.75246	118.18182	13.57141	118.18182	13.52542	118.18182	17.88391
121.21212	13.89037	121.21212	13.7677	121.21212	13.58861	121.21212	13.54315	121.21212	17.90186
124.24242	13.89981	124.24242	13.78222	124.24242	13.60517	124.24242	13.56025	124.24242	17.91918
127.27273	13.90884	127.27273	13.79607	127.27273	13.62112	127.27273	13.57676	127.27273	17.93589
130.30303	13.91747	130.30303	13.80928	130.30303	13.6365	130.30303	13.59269	130.30303	17.95202
133.33333	13.92574	133.33333	13.82189	133.33333	13.65132	133.33333	13.60807	133.33333	17.9676
136.36364	13.93366	136.36364	13.83392	136.36364	13.66561	136.36364	13.62293	136.36364	17.98265
139.39394	13.94125	139.39394	13.84542	139.39394	13.67938	139.39394	13.6373	139.39394	17.9972
142.42424	13.94852	142.42424	13.8564	142.42424	13.69268	142.42424	13.65118	142.42424	18.01126
145.45455	13.95549	145.45455	13.86689	145.45455	13.7055	145.45455	13.6646	145.45455	18.02485

148.48485	13.96217	148.48485	13.87693	148.48485	13.71788	148.48485	13.67758	148.48485	18.038
151.51515	13.96859	151.51515	13.88653	151.51515	13.72983	151.51515	13.69013	151.51515	18.05073
154.54546	13.97475	154.54546	13.89571	154.54546	13.74136	154.54546	13.70228	154.54546	18.06304
157.57576	13.98066	157.57576	13.90451	157.57576	13.7525	157.57576	13.71404	157.57576	18.07495
160.60606	13.98634	160.60606	13.91293	160.60606	13.76327	160.60606	13.72542	160.60606	18.08649
163.63636	13.9918	163.63636	13.921	163.63636	13.77366	163.63636	13.73643	163.63636	18.09766
166.66667	13.99705	166.66667	13.92874	166.66667	13.78371	166.66667	13.7471	166.66667	18.10847
169.69697	14.0021	169.69697	13.93616	169.69697	13.79342	169.69697	13.75743	169.69697	18.11895
172.72727	14.00697	172.72727	13.94328	172.72727	13.80281	172.72727	13.76743	172.72727	18.1291
175.75758	14.01165	175.75758	13.95012	175.75758	13.81189	175.75758	13.77713	175.75758	18.13894
178.78788	14.01615	178.78788	13.95668	178.78788	13.82067	178.78788	13.78652	178.78788	18.14847
181.81818	14.0205	181.81818	13.96299	181.81818	13.82917	181.81818	13.79563	181.81818	18.15772
184.84849	14.02469	184.84849	13.96905	184.84849	13.83739	184.84849	13.80445	184.84849	18.16668
187.87879	14.02873	187.87879	13.97488	187.87879	13.84535	187.87879	13.81301	187.87879	18.17537
190.90909	14.03262	190.90909	13.98049	190.90909	13.85305	190.90909	13.82131	190.90909	18.18379
193.93939	14.03638	193.93939	13.98589	193.93939	13.86051	193.93939	13.82936	193.93939	18.19197
196.9697	14.04002	196.9697	13.99109	196.9697	13.86773	196.9697	13.83717	196.9697	18.1999
200	14.04353	200	13.9961	200	13.87473	200	13.84475	200	18.2076
203.0303	14.04692	203.0303	14.00093	203.0303	13.88151	203.0303	13.8521	203.0303	18.21507
206.06061	14.0502	206.06061	14.00558	206.06061	13.88809	206.06061	13.85924	206.06061	18.22233
209.09091	14.05337	209.09091	14.01007	209.09091	13.89446	209.09091	13.86617	209.09091	18.22937
212.12121	14.05645	212.12121	14.0144	212.12121	13.90063	212.12121	13.8729	212.12121	18.23621
215.15151	14.05942	215.15151	14.01859	215.15151	13.90663	215.15151	13.87944	215.15151	18.24286
218.18182	14.0623	218.18182	14.02263	218.18182	13.91244	218.18182	13.88578	218.18182	18.24931
221.21212	14.06509	221.21212	14.02653	221.21212	13.91808	221.21212	13.89195	221.21212	18.25559
224.24242	14.06779	224.24242	14.0303	224.24242	13.92355	224.24242	13.89795	224.24242	18.26168
227.27273	14.07041	227.27273	14.03395	227.27273	13.92887	227.27273	13.90378	227.27273	18.26761
230.30303	14.07296	230.30303	14.03748	230.30303	13.93403	230.30303	13.90944	230.30303	18.27337
233.33333	14.07543	233.33333	14.0409	233.33333	13.93904	233.33333	13.91495	233.33333	18.27898
236.36364	14.07782	236.36364	14.04421	236.36364	13.94391	236.36364	13.92031	236.36364	18.28443
239.39394	14.08015	239.39394	14.04741	239.39394	13.94864	239.39394	13.92552	239.39394	18.28974
242.42424	14.08241	242.42424	14.05052	242.42424	13.95324	242.42424	13.93059	242.42424	18.2949
245.45455	14.08461	245.45455	14.05353	245.45455	13.95771	245.45455	13.93553	245.45455	18.29992
248.48485	14.08675	248.48485	14.05644	248.48485	13.96205	248.48485	13.94033	248.48485	18.30481
251.51515	14.08883	251.51515	14.05927	251.51515	13.96628	251.51515	13.94501	251.51515	18.30957
254.54546	14.09085	254.54546	14.06202	254.54546	13.9704	254.54546	13.94956	254.54546	18.31421
257.57576	14.09282	257.57576	14.06469	257.57576	13.9744	257.57576	13.954	257.57576	18.31873
260.60606	14.09473	260.60606	14.06728	260.60606	13.9783	260.60606	13.95832	260.60606	18.32313
263.63636	14.0966	263.63636	14.0698	263.63636	13.98209	263.63636	13.96253	263.63636	18.32742
266.66667	14.09842	266.66667	14.07224	266.66667	13.98578	266.66667	13.96664	266.66667	18.33159
269.69697	14.10019	269.69697	14.07462	269.69697	13.98938	269.69697	13.97064	269.69697	18.33567
272.72727	14.10192	272.72727	14.07693	272.72727	13.99289	272.72727	13.97454	272.72727	18.33964
275.75758	14.10361	275.75758	14.07918	275.75758	13.9963	275.75758	13.97834	275.75758	18.34352
278.78788	14.10525	278.78788	14.08137	278.78788	13.99963	278.78788	13.98205	278.78788	18.34729
281.81818	14.10686	281.81818	14.0835	281.81818	14.00288	281.81818	13.98567	281.81818	18.35098
284.84848	14.10843	284.84848	14.08558	284.84848	14.00605	284.84848	13.9892	284.84848	18.35458
287.87879	14.10996	287.87879	14.0876	287.87879	14.00913	287.87879	13.99265	287.87879	18.35809
290.90909	14.11146	290.90909	14.08957	290.90909	14.01215	290.90909	13.99601	290.90909	18.36152
293.93939	14.11292	293.93939	14.0915	293.93939	14.01509	293.93939	13.99929	293.93939	18.36486
296.9697	14.11435	296.9697	14.09337	296.9697	14.01796	296.9697	14.0025	296.9697	18.36813
300	14.11575	300	14.0952	300	14.02076	300	14.00563	300	18.37132