

## SUPPORTING INFORMATION

### **Engineering mononuclear Ln(III) complexes with a pseudo-macrocyclic hexadentate N<sub>4</sub>O<sub>2</sub> Schiff base ligand exhibiting slow magnetic relaxation.**

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**Table S1.-** Crystallographic data for complexes **1a – 4a**.

	<b>1a</b>	<b>2a</b>	<b>3a</b>	<b>4a</b>
<b>Formula</b>	C <sub>26.5</sub> H <sub>38.5</sub> Cl <sub>3</sub> YbN <sub>11.5</sub> O <sub>5.5</sub>	C <sub>26.5</sub> H <sub>38.5</sub> Cl <sub>3</sub> ErN <sub>11.5</sub> O <sub>5.5</sub>	C <sub>26.5</sub> H <sub>38.5</sub> Cl <sub>3</sub> DyN <sub>11.5</sub> O <sub>5.5</sub>	C <sub>26.5</sub> H <sub>38.5</sub> Cl <sub>3</sub> GdN <sub>11.5</sub> O <sub>5.5</sub>
<b>Molecular Weight (g·mol<sup>-1</sup>)</b>	885.58	879.80	875.04	869.79
<b>Crystal System</b>	Triclinico	Triclinico	Triclinico	Triclinico
<b>Space group</b>	P-1	P-1	P-1	P-1
<b>a (Å)</b>	10.4985(6)	10.5124(10)	10.5203(4)	10.5470(7)
<b>b (Å)</b>	10.8750(6)	10.8863(10)	10.8874(4)	10.8942(7)
<b>c (Å)</b>	17.0505(9)	17.0710(16)	17.0673(7)	17.1263(12)
<b>α (°)</b>	92.3069(16)	92.435(3)	92.2885(12)	92.2360(10)
<b>β (°)</b>	104.1952(14)	104.354(3)	104.6180(12)	105.0010(10)
<b>γ (°)</b>	110.5120(14)	110.487(3)	110.2182(12)	109.9570(10)
<b>Volume/Å<sup>3</sup></b>	1750.43(17)	1754.8(3)	1757.55(12)	1769.0(2)
<b>Z</b>	2	2	2	2
<b>D<sub>c</sub> (g·cm<sup>-3</sup>)</b>	1.680	1.665	1.653	1.633
<b>M (MoKα) (mm<sup>-1</sup>)</b>	2.955	2.675	13.939	2.156
<b>T (K)</b>	100	100.0	100	100.0
<b>Reflec. Collected/unique</b>	49766 / 10446	58847 / 7162	25302 / 5042	20639 (8019)
<b>R<sub>int</sub></b>	0.0404	0.0414	0.0501	0.0194
<b>Parameters</b>	449	449	449	479
<b>GOF on F<sup>2</sup></b>	1.084	1.093	1.047	1.057
<b>R<sub>1</sub><sup>a,b</sup></b>	0.0218 (0.0216)	0.0197 (0.0191)	0.0325 (0.0318)	0.0286 (0.0270)
<b>wR<sub>2</sub><sup>c</sup></b>	0.0534 (0.0532)	0.0481 (0.0478)	0.0813 (0.0805)	0.0697 (0.0685)
<b>Max. diff. peak /hole (e Å<sup>-3</sup>)</b>	1.39/-1.29	1.23/-0.81	1.49/-1.36	1.76/-0.90

<sup>a</sup>  $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$ . <sup>b</sup> Values in parentheses for reflections with  $I > 2\sigma(I)$ . <sup>c</sup>  $wR_2 = \{\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]\}^{1/2}$

**Table S2.-** Crystallographic data for complexes **1b** – **4b**.

	<b>1b</b>	<b>2b</b>	<b>3b</b>	<b>4b</b>
<b>Formula</b>	C <sub>50</sub> H <sub>47</sub> ClYbN <sub>8</sub> O <sub>10</sub>	C <sub>50</sub> H <sub>48</sub> ClErN <sub>8</sub> O <sub>10</sub>	C <sub>50.5</sub> H <sub>51</sub> ClDyN <sub>8</sub> O <sub>11</sub>	C <sub>49</sub> H <sub>49</sub> ClGdN <sub>8</sub> O <sub>11.5</sub>
<b>Molecular Weight (g·mol<sup>-1</sup>)</b>	1128.44	1123.67	1143.94	1126.66
<b>Crystal System</b>	Monoclínico	Monoclínico	Monoclínico	Monoclínico
<b>Space group</b>	Cc	Cc	Cc	Cc
<b>a (Å)</b>	18.3872(7)	18.439(4)	18.3856(11)	18.3873(9)
<b>b (Å)</b>	26.4704(10)	26.484(5)	26.3996(16)	26.1665(11)
<b>c (Å)</b>	13.0434(5)	13.068(5)	13.0842(8)	13.1228(11)
<b>α (°)</b>	90	90	90	90
<b>β (°)</b>	130.02	129.958(2)	129.8030(10)	129.4490(13)
<b>γ (°)</b>	90	90	90	90
<b>Volume/Å<sup>3</sup></b>	4861.9(3)	4892(2)	4878.9(5)	4875.4(5)
<b>Z</b>	4	4	4	4
<b>D<sub>c</sub> (g·cm<sup>-3</sup>)</b>	1.542	1.526	1.519	1.535
<b>M (MoKα) (mm<sup>-1</sup>)</b>	2.046	1.837	1.653	1.485
<b>T (K)</b>	273.15	273.15	100.0	100.0
<b>Reflec. Collected/unique</b>	15335 / 8774	15345 / 7132	28297 / 11151	30750 / 8548
<b>R<sub>int</sub></b>	0.0131	0.0242	0.0276	0.0202
<b>Parameters</b>	640	641	639	659
<b>GOF on F<sup>2</sup></b>	1.099	1.101	1.075	1.106
<b>R<sub>1</sub><sup>a,b</sup></b>	0.0346 (0.0339)	0.0392 (0.0378)	0.0417 (0.0390)	0.0206 (0.0200)
<b>wR<sub>2</sub><sup>c</sup></b>	0.0952 (0.0943)	0.1064 (0.1047)	0.1082 (0.1060)	0.0534 (0.0529)
<b>Max. diff. peak /hole (e Å<sup>-3</sup>)</b>	4.44/-0.61	3.63/-0.69	1.79/-0.46	1.67/-0.61

<sup>a</sup>  $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$ , <sup>b</sup> Values in parentheses for reflections with  $I > 2\sigma(I)$ , <sup>c</sup>  $wR_2 = [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$

**Table S3.** Selected bond angles (°) for complexes **1a** – **4a**.

	<b>1a</b>	<b>2a</b>	<b>3a</b>	<b>4a</b>
Cl2-Ln1-Cl1	144.181(15)	144.239(16)	144.22(3)	144.27(2)
Cl2-Ln1-N3	83.69(4)	84.06(4)	84.47(7)	84.97(5)
Cl2-Ln1-N5	76.42(3)	76.67(4)	76.47(7)	76.65(5)
O1-Ln1-Cl1	136.84(3)	136.70(4)	136.52(6)	136.35(4)
O1-Ln1-Cl2	74.78(4)	74.84(4)	75.10(6)	75.20(4)
O1-Ln1-N3	60.72(5)	60.72(5)	60.57(9)	60.56(6)
O1-Ln1-N4	120.34(5)	120.24(5)	119.79(9)	119.30(6)
O1-Ln1-N5	151.11(5)	151.43(5)	151.53(9)	151.83(6)
O1-Ln1-N6	109.86(5)	110.47(5)	111.28(9)	112.26(6)
O2-Ln1-Cl1	82.55(4)	82.74(4)	82.87(7)	83.30(5)
O2-Ln1-Cl2	104.78(4)	104.09(4)	103.45(7)	102.22(5)
O2-Ln1-O1	64.99(5)	65.13(5)	65.52(8)	65.76(6)
O2-Ln1-N3	120.24(5)	120.58(5)	121.10(9)	121.72(6)
O2-Ln1-N4	165.27(5)	165.78(5)	166.58(10)	168.04(7)
O2-Ln1-N5	121.31(5)	121.03(5)	120.72(9)	120.38(6)
O2-Ln1-N6	62.76(5)	62.57(5)	62.26(9)	61.84(6)
O3-Ln1-Cl1	74.34(4)	74.23(4)	74.11(7)	74.08(5)
O3-Ln1-Cl2	141.26(4)	141.36(4)	141.53(7)	141.56(5)
O3-Ln1-O1	72.08(5)	71.88(5)	71.47(9)	71.02(7)
O3-Ln1-O2	78.71(5)	79.09(5)	79.50(10)	80.20(7)
O3-Ln1-N3	62.85(5)	62.80(5)	62.81(10)	62.77(7)
O3-Ln1-N4	89.81(5)	90.01(6)	90.46(10)	91.15(7)
O3-Ln1-N5	135.41(5)	135.28(5)	135.48(10)	135.51(7)
O3-Ln1-N6	133.53(5)	133.36(5)	133.18(10)	132.87(7)
N3-Ln1-Cl1	123.41(4)	123.12(4)	122.80(7)	122.42(5)
N3-Ln1-N5	118.20(5)	118.15(5)	117.90(10)	117.56(7)
N4-Ln1-Cl1	85.51(4)	85.54(4)	85.85(7)	86.40(5)
N4-Ln1-Cl2	89.95(4)	90.13(4)	89.95(7)	89.69(5)
N4-Ln1-N3	60.45(5)	60.37(5)	60.12(10)	59.75(7)
N4-Ln1-N5	61.67(5)	61.52(5)	61.36(10)	61.03(7)
N5-Ln1-Cl1	70.17(3)	70.10(4)	70.37(7)	70.44(5)
N6-Ln1-Cl1	75.77(4)	75.46(4)	75.21(7)	74.68(5)
N6-Ln1-Cl2	76.88(4)	76.95(4)	76.95(7)	77.12(5)
N6-Ln1-N3	160.25(5)	160.78(5)	161.26(10)	162.02(7)
N6-Ln1-N4	122.29(5)	121.90(5)	121.52(10)	120.98(7)
N6-Ln1-N5	60.62(5)	60.38(5)	60.16(9)	59.95(7)

**Table S4.** Selected bond angles (°) for complexes **1b** – **4b**.

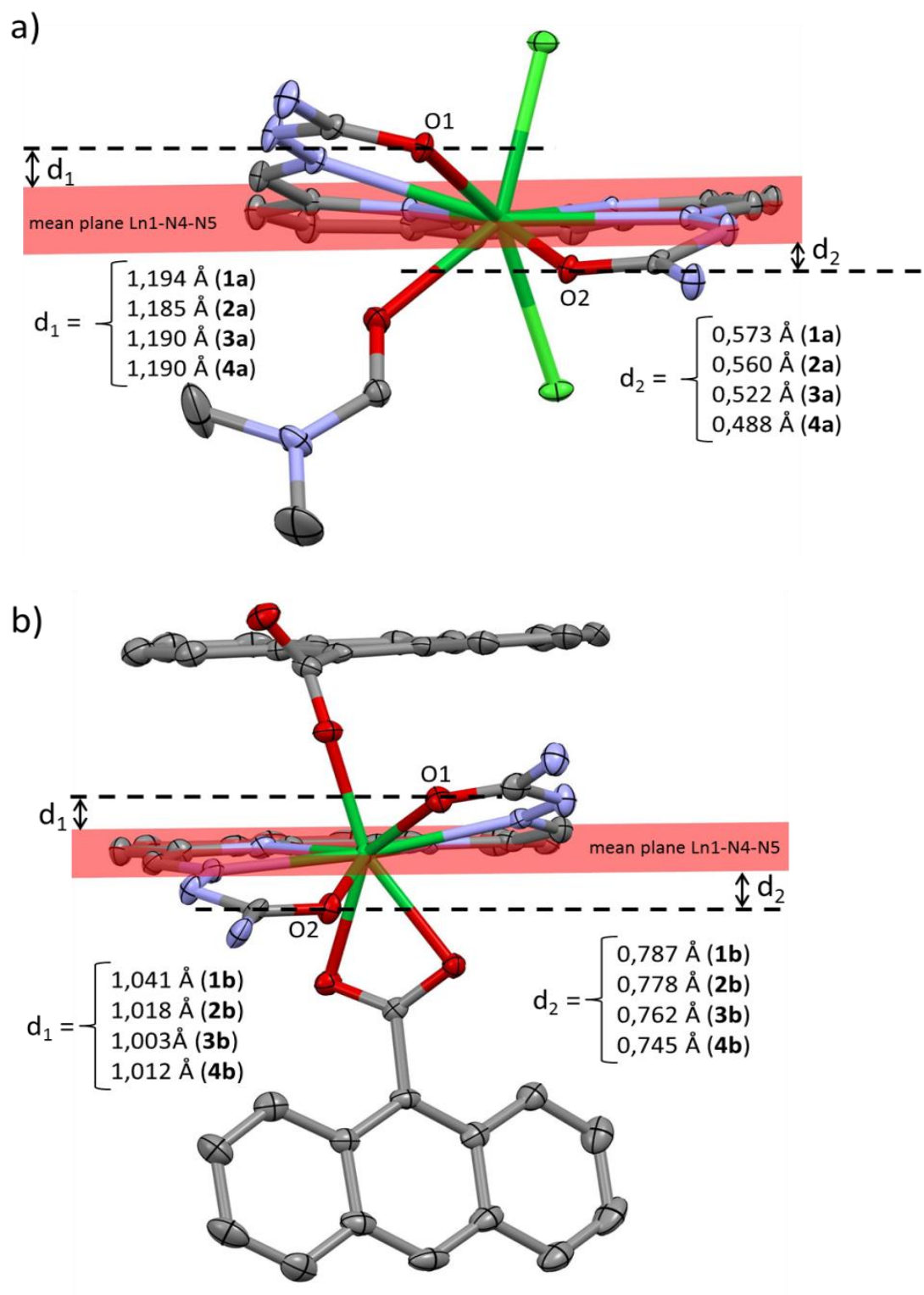
	<b>1b</b>	<b>2b</b>	<b>3b</b>	<b>4b</b>
O1-Ln1-N3	61.1(2)	60.7(2)	60.4(2)	60.25(13)
O1-Ln1-N4	121.0(2)	120.6(3)	120.0(3)	119.35(15)
O1-Ln1-N5	153.6(2)	154.5(3)	155.2(2)	155.17(14)
O1-Ln1-N6	110.5(3)	111.4(3)	112.5(3)	113.64(15)
O2-Ln1-O1	64.00(16)	64.09(19)	64.65(18)	65.37(11)
O2-Ln1-N3	113.9(2)	114.1(2)	115.1(2)	115.71(13)
O2-Ln1-N4	159.2(2)	159.7(2)	160.5(2)	161.00(14)
O2-Ln1-N5	122.2(2)	122.1(3)	121.7(2)	121.39(14)
O2-Ln1-N6	62.5(2)	62.5(3)	61.8(3)	61.49(15)
O3-Ln1-O1	88.1(2)	87.8(2)	87.5(2)	87.66(13)
O3-Ln1-O2	76.79(19)	77.4(2)	78.0(2)	78.71(12)
O3-Ln1-N3	67.6(2)	67.7(3)	68.0(3)	67.76(16)
O3-Ln1-N4	83.1(2)	83.0(2)	83.1(2)	83.04(13)
O3-Ln1-N5	118.1(2)	117.5(2)	116.9(2)	116.71(13)
O3-Ln1-N6	118.1(2)	117.9(3)	117.1(2)	116.45(15)
O4-Ln1-O1	133.4(2)	132.8(2)	132.5(2)	133.38(13)
O4-Ln1-O2	79.3(2)	79.6(2)	79.8(2)	81.01(13)
O4-Ln1-O3	54.77(18)	54.1(2)	53.68(19)	53.39(12)
O4-Ln1-N3	116.0(2)	115.6(3)	115.3(2)	114.22(15)
O4-Ln1-N4	84.8(2)	84.8(2)	84.9(2)	83.92(13)
O4-Ln1-N5	70.8(2)	70.9(2)	70.7(2)	70.32(13)
O4-Ln1-N6	72.6(2)	72.7(3)	72.2(2)	72.10(15)
O5-Ln1-O1	75.1(2)	75.7(2)	76.3(2)	75.47(14)
O5-Ln1-O2	106.1(2)	105.5(2)	104.5(2)	101.65(13)
O5-Ln1-O3	158.9(2)	159.4(2)	160.1(2)	160.90(11)
O5-Ln1-O4	146.2(2)	146.3(2)	146.1(2)	145.71(14)
O5-Ln1-N3	92.7(3)	93.1(3)	93.6(3)	95.62(19)
O5-Ln1-N4	94.6(2)	94.7(3)	95.0(2)	97.32(14)
O5-Ln1-N5	78.7(2)	78.8(3)	79.0(2)	79.71(14)
O5-Ln1-N6	80.4(3)	80.3(3)	80.3(3)	79.23(18)
N4-Ln1-N3	61.6(2)	61.6(2)	61.2(2)	60.82(14)
N4-Ln1-N5	63.61(19)	63.4(2)	63.1(2)	63.07(13)
N5-Ln1-N3	123.5(2)	123.3(2)	122.8(2)	122.49(13)
N6-Ln1-N3	170.5(2)	171.0(3)	171.8(3)	173.11(19)
N6-Ln1-N4	125.1(3)	124.7(3)	124.5(3)	124.07(16)
N6-Ln1-N5	61.8(3)	61.6(3)	61.7(3)	61.41(15)

**Table S5.** Selected bond distances for the complexes **1a – 4a** and **1b – 4b** (Å).

	<b>1a</b>	<b>2a</b>	<b>3a</b>	<b>4a</b>
Ln1-O1	2.527(1)	2.531(1)	2.536(3)	2.551(2)
Ln1-O2	2.342(1)	2.351(1)	2.372(3)	2.391(2)
Ln1-O3	2.322(1)	2.350(2)	2.372(3)	2.406(2)
Ln1-N3	2.613(2)	2.614(2)	2.625(3)	2.639(2)
Ln1-N4	2.586(2)	2.594(2)	2.611(3)	2.633(2)
Ln1-N5	2.623(2)	2.633(2)	2.641(3)	2.668(2)
Ln1-N6	2.528(1)	2.577(2)	2.595(3)	2.614(2)
Ln1-Cl1	2.669(1)	2.669(1)	2.702(1)	2.731(1)
Ln1-Cl2	2.608(1)	2.608(1)	2.649(1)	2.683(1)
	<b>1b</b>	<b>2b</b>	<b>3b</b>	<b>4b</b>
Ln1-O1	2.452(7)	2.452(8)	2.467(7)	2.466(4)
Ln1-O2	2.386(6)	2.405(7)	2.414(6)	2.418(4)
Ln1-O3	2.382(5)	2.414(6)	2.423(6)	2.448(3)
Ln1-O4	2.373(5)	2.406(6)	2.419(5)	2.444(3)
Ln1-O5	2.170(7)	2.214(8)	2.224(8)	2.301(5)
Ln1-N3	2.564(10)	2.583(12)	2.597(10)	2.613(6)
Ln1-N4	2.538(8)	2.550(9)	2.573(9)	2.581(5)
Ln1- N5	2.551(8)	2.564(8)	2.573(8)	2.593(5)
Ln1- N6	2.525(10)	2.526(11)	2.562(10)	2.579(6)

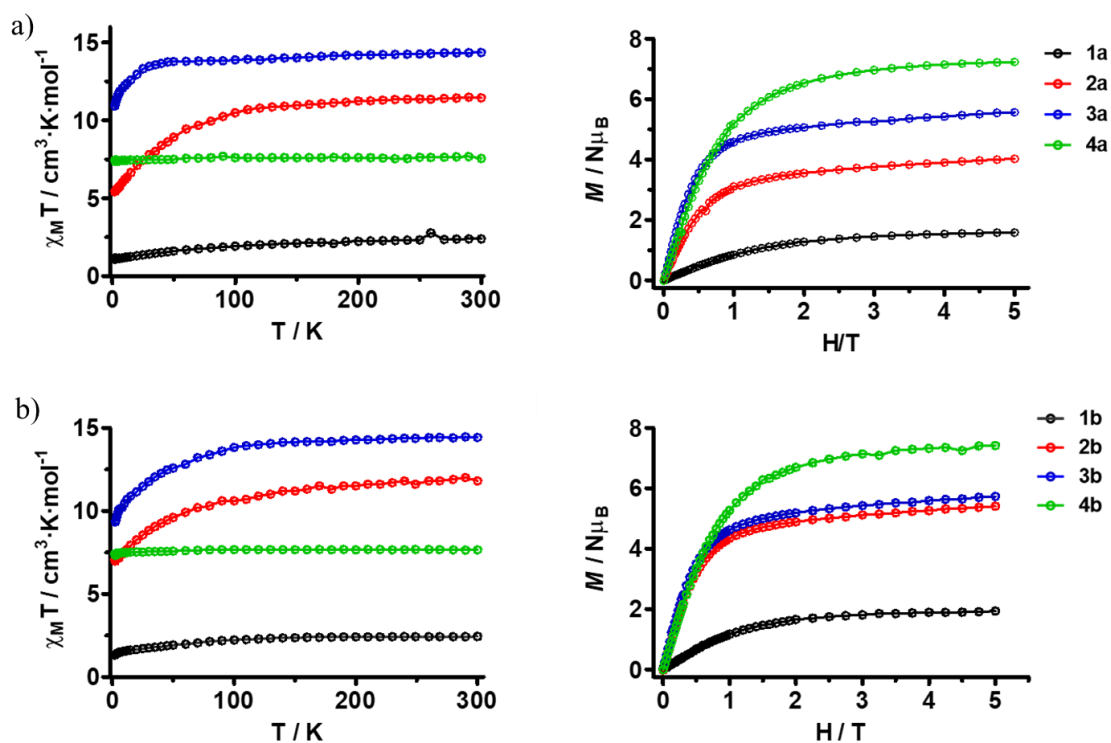
**Table S6.** Continuous Shape Measures of the coordination sphere geometry for the Ln<sup>III</sup> centres in the complexes described in this work.

Compound	MFF	HH	JTDIC	JCTPR	JTCTPR	CSAPR	JCSAPR	CCU	JCCU	JTC	HBPY	OPY	EP
1a	3.773	3.787	12.715	5.603	5.880	4.762	6.184	5.355	7.040	15.138	13.946	20.938	31.807
2a	3.880	3.688	12.743	5.764	6.069	4.895	6.335	5.356	7.054	15.077	13.835	20.935	31.835
3a	4.025	3.577	12.740	5.982	6.261	5.077	6.511	5.340	7.051	15.01	13.710	20.953	31.749
4a	4.252	3.446	12.728	6.345	6.591	5.385	6.866	5.348	7.061	15.092	13.524	20.849	31.655
1b	4.901	4.045	10.172	6.372	6.615	6.049	6.729	3.895	5.140	14.080	14.280	24.471	33.112
2b	5.023	3.853	10.023	6.532	6.808	6.240	6.946	3.906	5.190	14.121	14.225	24.432	33.058
3b	5.307	3.705	9.858	6.945	7.208	6.666	7.397	3.912	5.246	14.073	14.022	24.412	32.975
4b	5.528	3.559	9.642	7.260	7.683	7.131	7.880	3.846	5.229	13.707	13.963	24.429	32.321
MFF-9	13 Cs	Muffin					CCU-9	6 C4v	Spherical-relaxed capped cube				
HH-9	12 C2v	Hula-hoop					JCCU-9	5 C4v	Capped cube J8				
JTDIC-9	11 C3v	Tridiminished icosahedron J63					JTC-9	4 C3v	Johnson triangular cupola J3				
TCTPR-9	10 D3h	Spherical tricapped trigonal prism					HBPY-9	3 D7h	Heptagonal bipyramid				
JTCTPR-9	9 D3h	Tricapped trigonal prism J51					OPY-9	2 C8v	Octagonal pyramid				
CSAPR-9	8 C4v	Spherical capped square antiprism					EP-9	1 D9h	Enneagon				
JCSAPR-9	7 C4v	Capped square antiprism J10											

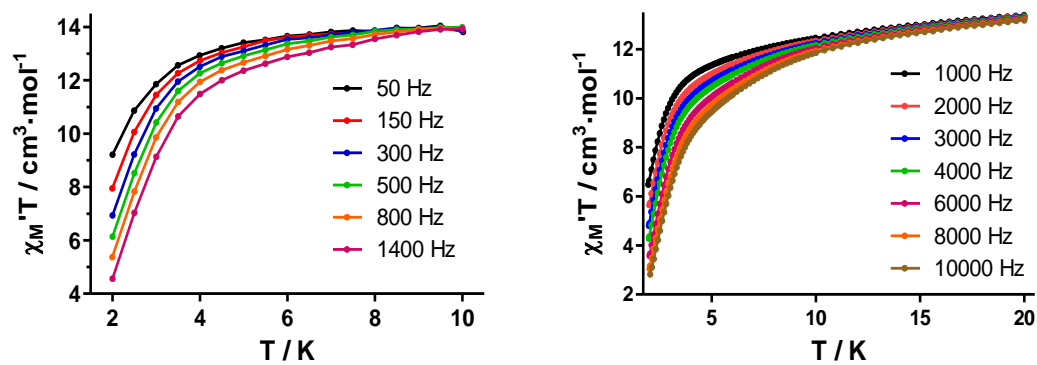


**Figure S1.** Molecular plane containing atoms Ln1-N4-N5, as well as the distance from the O1 and O2 atoms in complexes **1a-4a** and **1b-4b**.





**Figure S2.** Thermal dependence of the  $\chi_M T$  product between 2 K – 300 K (left) and field dependence of the magnetization at  $T = 2$  K (right) for complexes **1a-4a** (a) and **1b-4b** (b). Solid lines are a guide for the eye.



**Figure S3.-** Thermal dependence of the in-phase  $\chi_M' T$  under 1000 Oe dc field for complex **3a** (left) and **3b** (right).

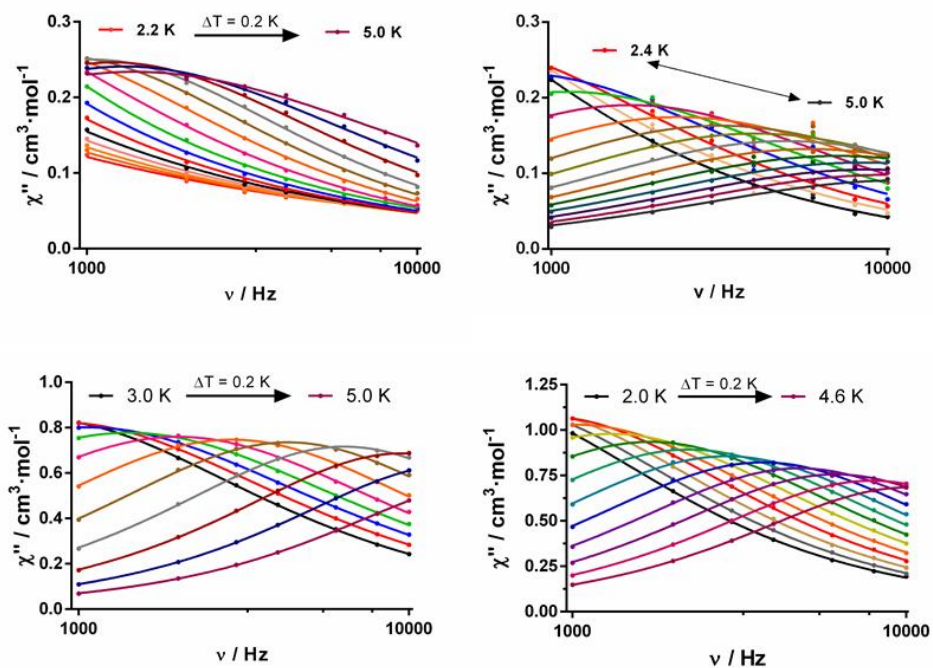


Figure S4.- Frequency dependence of the out-of-phase ac signal ( $\chi_M''$ ) for compounds **1a** (top left), **1v** (top right), **2a** (down, left), **2b** (down, right). Solid lines represent the best fits to the Debye model.

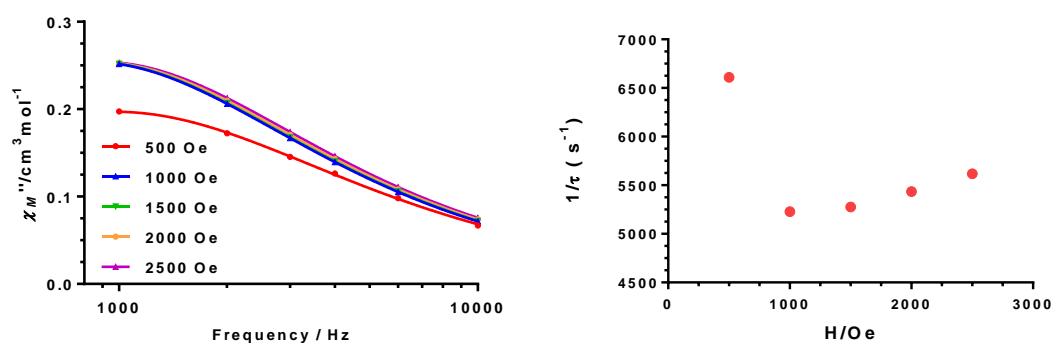


Figure S5.- Frequency dependence of the ( $\chi_M''$ ) signal at the indicated fields (left) and field dependence of  $\tau^{-1}$  (right) for compound **1a**.

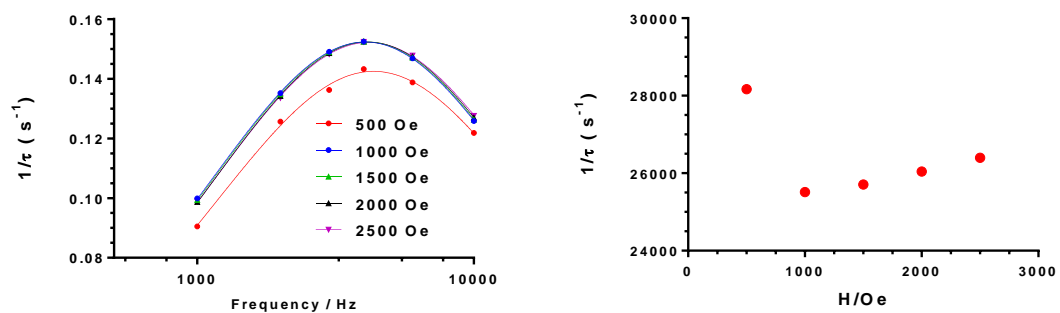


Figure S6.- Frequency dependence of the ( $\chi_M''$ ) signal at the indicated fields (left) and field dependence of  $\tau^{-1}$  (right) for compound 1b.

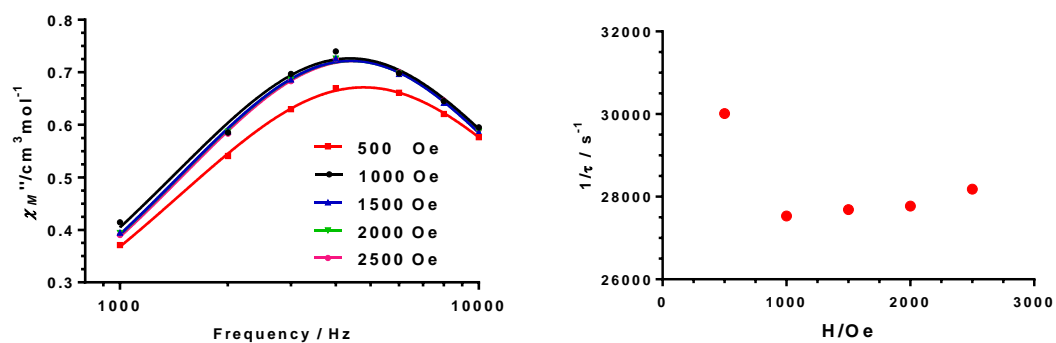


Figure S7.- Frequency dependence of the ( $\chi_M''$ ) signal at the indicated fields (left) and field dependence of  $\tau^{-1}$  (right) for compound 2a.

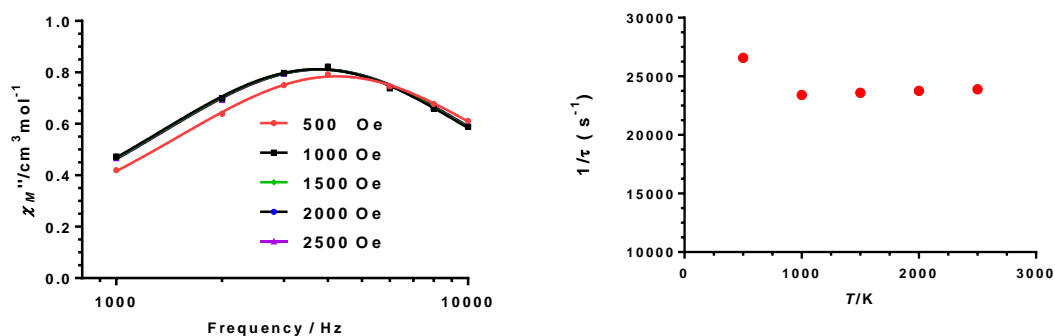


Figure S8.- Frequency dependence of the ( $\chi_M''$ ) signal at the indicated fields (left) and field dependence of  $\tau^{-1}$  (right) for compound 2a.

**Table S7.** CASSCF energies of the first 4 KDs and their g-values.

Complex 1a	$\Delta$ (cm <sup>-1</sup> )	$g_{xx}$ , $g_{yy}$ , $g_{zz}$
Ground	0.0	0.07, 0.12, 7.68
1 <sup>st</sup> excited	216.8	0.98, 1.65, 5.39
2 <sup>nd</sup> excited	300.6	4.34, 2.68, 0.19
3 <sup>rd</sup> excited	488.1	0.79, 1.23, 6.95
Complex 1b	$\Delta$ (cm <sup>-1</sup> )	$g_{xx}$ , $g_{yy}$ , $g_{zz}$
Ground	0.0	0.51, 1.11, 7.16
1 <sup>st</sup> excited	257.9	2.21, 2.55, 4.36
2 <sup>nd</sup> excited	451.44	1.47, 2.12, 4.30
3 <sup>rd</sup> excited	628.0	1.62, 2.12, 6.04
Complex 2a	$\Delta$ (cm <sup>-1</sup> )	$g_{xx}$ , $g_{yy}$ , $g_{zz}$
Ground	0.0	0.43, 0.71, 15.81
1 <sup>st</sup> excited	54.6	2.63, 2.88, 11.56
2 <sup>nd</sup> excited	105.2	1.13, 4.96, 9.78
3 <sup>rd</sup> excited	195.4	1.18, 3.13, 8.90
Complex 2b	$\Delta$ (cm <sup>-1</sup> )	$g_{xx}$ , $g_{yy}$ , $g_{zz}$
Ground	0.0	0.74, 1.34, 14.52
1 <sup>st</sup> excited	54.1	2.65, 3.43, 10.51
2 <sup>nd</sup> excited	125.8	7.63, 7.02, 0.28
3 <sup>rd</sup> excited	252.0	6.48, 3.46, 0.27
Complex 3a	$\Delta$ (cm <sup>-1</sup> )	$g_{xx}$ , $g_{yy}$ , $g_{zz}$
Ground	0.0	0.17, 0.36, 19.43

<b>1<sup>st</sup> excited</b>	118.3	2.07, 4.98, 13.04
<b>2<sup>nd</sup> excited</b>	163.3	3.73, 4.2, 9.57
<b>3<sup>rd</sup> excited</b>	226.5	0.20, 0.83, 12.42

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<b>Complex 3b</b>	<b><math>\Delta</math> (cm<sup>-1</sup>)</b>	<b><math>g_{xx}</math>, <math>g_{yy}</math>, <math>g_{zz}</math></b>
<b>Ground</b>	0.0	0.03, 0.04, 19.81
<b>1<sup>st</sup> excited</b>	241.7	0.95, 2.02, 15.92
<b>2<sup>nd</sup> excited</b>	328.7	4.37, 5.38, 10.79
<b>3<sup>rd</sup> excited</b>	395.9	1.13, 2.42, 11.70

**Table S8.** Calculated at CASSCF level the Crystal-Field Hamiltonian data for all the studied complexes.

<b>B(k,q)</b>							
<b>k</b>	<b>q</b>	<b>1a</b>	<b>1b</b>	<b>2a</b>	<b>2b</b>	<b>3a</b>	<b>3b</b>
2	-2	5.78E+00	-5.91E+00	-2.03E-01	1.09E+00	-9.47E-01	-4.45E-02
2	-1	-9.62E-01	2.48E+00	-3.22E-01	-1.29E+00	-9.46E-02	1.51E-01
2	0	-9.48E+00	-1.13E+01	-7.89E-01	-6.73E-01	-1.60E+00	-2.74E+00
2	1	-1.04E+01	5.58E+00	-5.66E-01	2.34E-01	2.89E+00	1.21E+00
2	2	7.76E+00	1.68E+01	6.57E-01	1.19E+00	1.77E+00	1.81E+00
4	-4	6.17E-03	-2.96E-02	-5.33E-05	1.83E-02	-2.64E-03	-7.38E-04
4	-3	5.27E-02	3.24E-01	-1.96E-02	-5.62E-02	1.41E-03	3.27E-02
4	-2	2.76E-01	-2.40E-01	-7.79E-03	-3.52E-03	1.92E-03	6.49E-03
4	-1	4.44E-02	2.93E-02	6.46E-03	5.32E-03	1.97E-03	8.86E-03
4	0	-6.98E-02	-8.41E-02	1.24E-03	1.23E-03	-3.58E-03	-6.47E-03
4	1	4.90E-01	-3.26E-01	-1.52E-02	1.43E-03	-1.04E-02	-6.59E-03
4	2	1.09E-01	3.92E-01	-8.41E-03	-7.94E-03	1.83E-02	1.32E-02
4	3	-3.61E-01	6.35E-02	1.34E-02	4.35E-03	2.95E-02	1.66E-02
4	4	-2.87E-02	-3.65E-01	2.04E-03	4.11E-03	-6.61E-03	-1.93E-03
6	-6	-6.87E-03	3.33E-02	3.54E-05	-5.22E-05	5.17E-04	6.72E-04
6	-5	-2.06E-02	-3.83E-02	-8.68E-05	4.54E-06	-2.49E-04	-5.27E-05
6	-4	4.42E-03	-9.75E-03	-2.28E-05	2.06E-04	-2.31E-05	1.79E-05
6	-3	1.96E-02	4.93E-02	3.64E-04	1.04E-04	1.07E-04	-2.26E-06

6	-2	-1.26E-02	-3.86E-04	-5.28E-05	6.92E-05	-3.39E-05	-1.45E-04
6	-1	3.17E-02	4.12E-02	-5.64E-05	-4.90E-04	1.48E-05	-1.83E-04
6	0	-1.49E-03	3.95E-04	-5.75E-05	8.93E-05	-6.49E-06	-5.38E-06
6	1	-1.89E-02	1.35E-02	1.05E-04	2.25E-04	-8.35E-05	-7.83E-06
6	2	5.74E-03	1.68E-02	-4.28E-04	2.18E-04	-4.85E-05	-1.27E-04
6	3	-3.86E-02	3.10E-02	5.00E-04	5.80E-05	5.02E-05	8.39E-05
6	4	2.18E-03	8.87E-03	-1.61E-04	1.83E-04	8.15E-05	5.91E-05
6	5	9.17E-03	-2.75E-02	-2.96E-04	1.40E-03	-1.27E-04	-2.55E-04
6	6	5.13E-03	4.33E-03	-1.35E-04	-1.61E-04	2.55E-04	-8.22E-05

**Table S9.** Calculated CASSCF  $\chi T$  ( $\text{cm}^3\text{K}^{-1}\text{mol}^{-1}$ ) vs. T (K) data for all the complexes

T (K)	$\chi T$ ( $\text{cm}^3\text{K}^{-1}\text{mol}^{-1}$ )					
	1a	1b	2a	2b	3a	3b
0	1.84628	1.65019	7.83153	6.66443	11.8061	12.2757
1	1.85036	1.6547	7.88887	6.73109	11.8306	12.2856
2	1.85444	1.65922	7.94621	6.79777	11.855	12.2955
3	1.85852	1.66373	8.00355	6.86444	11.8795	12.3054
4	1.8626	1.66824	8.06089	6.93111	11.9039	12.3153
5	1.86668	1.67275	8.11823	6.99778	11.9284	12.3251
6	1.87076	1.67727	8.17557	7.06446	11.9528	12.335
7	1.87483	1.68178	8.23287	7.13112	11.9773	12.3449
8	1.87891	1.68629	8.29008	7.19777	12.0017	12.3548
9	1.88299	1.69081	8.34708	7.26437	12.0262	12.3647
10	1.88707	1.69532	8.4037	7.33086	12.0506	12.3745
11	1.89115	1.69983	8.45975	7.39714	12.0751	12.3844
12	1.89523	1.70435	8.51503	7.46311	12.0995	12.3943
13	1.89931	1.70886	8.56935	7.52863	12.124	12.4042
14	1.90339	1.71337	8.62256	7.59358	12.1484	12.414
15	1.90747	1.71789	8.67452	7.65783	12.1728	12.4239
16	1.91155	1.7224	8.72514	7.72125	12.1972	12.4338

17	1.91563	1.72691	8.77437	7.78375	12.2216	12.4437
18	1.91971	1.73142	8.82218	7.84523	12.2459	12.4536
19	1.92379	1.73594	8.86854	7.90563	12.2702	12.4634
20	1.92787	1.74045	8.91348	7.96487	12.2944	12.4733
21	1.93195	1.74496	8.95702	8.02292	12.3185	12.4832
22	1.93603	1.74948	8.99919	8.07975	12.3424	12.4931
23	1.94011	1.75399	9.04003	8.13534	12.3663	12.503
24	1.94419	1.7585	9.07959	8.18968	12.39	12.5128
25	1.94826	1.76302	9.11792	8.24277	12.4135	12.5227
26	1.95234	1.76753	9.15507	8.29462	12.4368	12.5326
27	1.95642	1.77204	9.19109	8.34523	12.4599	12.5425
28	1.9605	1.77655	9.22604	8.39462	12.4828	12.5523
29	1.96457	1.78107	9.25997	8.44281	12.5054	12.5622
30	1.96865	1.78558	9.29293	8.48982	12.5278	12.5721
31	1.97272	1.79009	9.32496	8.53569	12.55	12.5819
32	1.97679	1.7946	9.35612	8.58043	12.5718	12.5918
33	1.98086	1.79911	9.38644	8.62407	12.5934	12.6017
34	1.98492	1.80362	9.41598	8.66664	12.6147	12.6115
35	1.98898	1.80813	9.44476	8.70817	12.6357	12.6214
36	1.99304	1.81263	9.47283	8.7487	12.6564	12.6312
37	1.99709	1.81714	9.50023	8.78825	12.6768	12.641
38	2.00114	1.82164	9.52698	8.82684	12.6969	12.6508
39	2.00519	1.82614	9.55312	8.86452	12.7167	12.6606
40	2.00922	1.83064	9.57868	8.90132	12.7361	12.6704
41	2.01325	1.83513	9.60369	8.93725	12.7553	12.6802
42	2.01728	1.83962	9.62817	8.97235	12.7742	12.6899
43	2.02129	1.8441	9.65215	9.00665	12.7927	12.6997
44	2.0253	1.84858	9.67565	9.04017	12.811	12.7094
45	2.0293	1.85306	9.69869	9.07295	12.8289	12.7191
46	2.03329	1.85753	9.72129	9.105	12.8465	12.7287
47	2.03727	1.86199	9.74347	9.13636	12.8639	12.7384
48	2.04124	1.86645	9.76524	9.16704	12.8809	12.748
49	2.0452	1.87089	9.78663	9.19707	12.8977	12.7575
50	2.04914	1.87534	9.80765	9.22647	12.9141	12.7671
51	2.05308	1.87977	9.82831	9.25527	12.9303	12.7766
52	2.057	1.88419	9.84863	9.28348	12.9462	12.7861
53	2.06091	1.8886	9.86861	9.31112	12.9618	12.7955
54	2.0648	1.893	9.88827	9.33822	12.9772	12.8049

55	2.06868	1.89739	9.90762	9.36479	12.9923	12.8142
56	2.07254	1.90177	9.92667	9.39085	13.0071	12.8236
57	2.07639	1.90614	9.94543	9.41642	13.0217	12.8328
58	2.08023	1.91049	9.9639	9.44151	13.036	12.8421
59	2.08404	1.91483	9.9821	9.46613	13.05	12.8512
60	2.08784	1.91915	10	9.49031	13.0638	12.8604
61	2.09162	1.92347	10.0177	9.51406	13.0774	12.8695
62	2.09539	1.92776	10.0351	9.53739	13.0908	12.8785
63	2.09914	1.93204	10.0523	9.5603	13.1039	12.8875
64	2.10286	1.93631	10.0692	9.58283	13.1167	12.8964
65	2.10657	1.94055	10.0859	9.60497	13.1294	12.9053
66	2.11026	1.94478	10.1023	9.62673	13.1418	12.9141
67	2.11393	1.94899	10.1185	9.64814	13.154	12.9229
68	2.11758	1.95319	10.1345	9.66919	13.166	12.9317
69	2.12122	1.95737	10.1503	9.6899	13.1778	12.9403
70	2.12483	1.96152	10.1658	9.71028	13.1894	12.9489
71	2.12841	1.96566	10.1812	9.73033	13.2008	12.9575
72	2.13198	1.96978	10.1963	9.75007	13.212	12.966
73	2.13553	1.97388	10.2112	9.7695	13.223	12.9745
74	2.13905	1.97795	10.226	9.78863	13.2338	12.9829
75	2.14256	1.98201	10.2405	9.80746	13.2444	12.9912
76	2.14604	1.98605	10.2548	9.82601	13.2548	12.9995
77	2.1495	1.99006	10.2689	9.84429	13.2651	13.0077
78	2.15293	1.99405	10.2829	9.86229	13.2752	13.0159
79	2.15635	1.99802	10.2966	9.88002	13.2851	13.024
80	2.15974	2.00197	10.3102	9.89749	13.2949	13.032
81	2.16311	2.0059	10.3236	9.91471	13.3045	13.04
82	2.16645	2.0098	10.3368	9.93167	13.3139	13.0479
83	2.16977	2.01369	10.3498	9.9484	13.3231	13.0558
84	2.17307	2.01755	10.3627	9.96488	13.3322	13.0636
85	2.17634	2.02138	10.3754	9.98113	13.3412	13.0714
86	2.1796	2.02519	10.3879	9.99715	13.35	13.0791
87	2.18282	2.02898	10.4002	10.0129	13.3587	13.0867
88	2.18603	2.03275	10.4124	10.0285	13.3672	13.0943
89	2.18921	2.03649	10.4244	10.0439	13.3755	13.1018
90	2.19236	2.04021	10.4362	10.059	13.3838	13.1093
91	2.19549	2.0439	10.4479	10.0739	13.3919	13.1167
92	2.1986	2.04757	10.4594	10.0887	13.3998	13.1241



93	2.20169	2.05122	10.4708	10.1032	13.4077	13.1314
94	2.20475	2.05484	10.482	10.1175	13.4154	13.1386
95	2.20778	2.05844	10.4931	10.1317	13.4229	13.1458
96	2.21079	2.06202	10.504	10.1456	13.4304	13.1529
97	2.21378	2.06557	10.5147	10.1594	13.4377	13.16
98	2.21675	2.06909	10.5253	10.1729	13.4449	13.167
99	2.21969	2.0726	10.5358	10.1863	13.452	13.174
100	2.2226	2.07607	10.5461	10.1995	13.459	13.1809
101	2.22549	2.07953	10.5563	10.2126	13.4659	13.1877
102	2.22836	2.08296	10.5663	10.2254	13.4726	13.1945
103	2.2312	2.08636	10.5762	10.2381	13.4793	13.2013
104	2.23402	2.08975	10.5859	10.2506	13.4858	13.2079
105	2.23682	2.0931	10.5956	10.263	13.4923	13.2146
106	2.23959	2.09644	10.6051	10.2752	13.4986	13.2211
107	2.24234	2.09975	10.6144	10.2872	13.5048	13.2277
108	2.24507	2.10303	10.6236	10.2991	13.511	13.2341
109	2.24777	2.1063	10.6327	10.3108	13.517	13.2406
110	2.25045	2.10953	10.6417	10.3224	13.523	13.2469
111	2.2531	2.11275	10.6505	10.3338	13.5288	13.2532
112	2.25573	2.11594	10.6593	10.345	13.5346	13.2595
113	2.25834	2.11911	10.6679	10.3562	13.5402	13.2657
114	2.26093	2.12225	10.6764	10.3671	13.5458	13.2719
115	2.26349	2.12537	10.6847	10.378	13.5513	13.278
116	2.26603	2.12847	10.693	10.3887	13.5567	13.284
117	2.26855	2.13155	10.7011	10.3992	13.5621	13.29
118	2.27104	2.1346	10.7091	10.4096	13.5673	13.296
119	2.27351	2.13763	10.717	10.4199	13.5725	13.3019
120	2.27596	2.14063	10.7248	10.4301	13.5775	13.3077
121	2.27839	2.14361	10.7325	10.4401	13.5826	13.3136
122	2.28079	2.14658	10.7401	10.45	13.5875	13.3193
123	2.28318	2.14951	10.7475	10.4597	13.5924	13.325
124	2.28554	2.15243	10.7549	10.4694	13.5971	13.3307
125	2.28788	2.15532	10.7622	10.4789	13.6019	13.3363
126	2.29019	2.15819	10.7693	10.4883	13.6065	13.3419
127	2.29249	2.16104	10.7764	10.4976	13.6111	13.3474
128	2.29476	2.16387	10.7834	10.5067	13.6156	13.3529
129	2.29702	2.16667	10.7902	10.5158	13.62	13.3583
130	2.29925	2.16946	10.797	10.5247	13.6244	13.3637

131	2.30146	2.17222	10.8037	10.5335	13.6287	13.369
132	2.30365	2.17496	10.8103	10.5422	13.6329	13.3743
133	2.30582	2.17768	10.8168	10.5508	13.6371	13.3795
134	2.30797	2.18037	10.8232	10.5593	13.6412	13.3847
135	2.3101	2.18305	10.8295	10.5677	13.6453	13.3899
136	2.31221	2.18571	10.8357	10.5759	13.6493	13.395
137	2.3143	2.18834	10.8418	10.5841	13.6533	13.4001
138	2.31637	2.19096	10.8479	10.5922	13.6572	13.4051
139	2.31842	2.19355	10.8539	10.6001	13.661	13.4101
140	2.32045	2.19612	10.8598	10.608	13.6648	13.415
141	2.32246	2.19868	10.8656	10.6157	13.6685	13.4199
142	2.32445	2.20121	10.8713	10.6234	13.6722	13.4248
143	2.32642	2.20372	10.8769	10.631	13.6758	13.4296
144	2.32838	2.20622	10.8825	10.6385	13.6793	13.4343
145	2.33031	2.20869	10.888	10.6458	13.6829	13.4391
146	2.33223	2.21115	10.8934	10.6531	13.6863	13.4437
147	2.33413	2.21358	10.8988	10.6603	13.6898	13.4484
148	2.33601	2.216	10.9041	10.6675	13.6931	13.453
149	2.33787	2.21839	10.9093	10.6745	13.6965	13.4576
150	2.33971	2.22077	10.9144	10.6814	13.6997	13.4621
151	2.34154	2.22313	10.9194	10.6883	13.703	13.4666
152	2.34334	2.22547	10.9244	10.695	13.7062	13.471
153	2.34513	2.22779	10.9294	10.7017	13.7093	13.4754
154	2.34691	2.23009	10.9342	10.7083	13.7124	13.4798
155	2.34866	2.23238	10.939	10.7148	13.7155	13.4841
156	2.3504	2.23464	10.9437	10.7213	13.7185	13.4884
157	2.35213	2.23689	10.9484	10.7276	13.7215	13.4926
158	2.35383	2.23912	10.953	10.7339	13.7244	13.4969
159	2.35552	2.24133	10.9576	10.7401	13.7273	13.501
160	2.35719	2.24353	10.962	10.7463	13.7302	13.5052
161	2.35885	2.2457	10.9665	10.7523	13.733	13.5093
162	2.36049	2.24786	10.9708	10.7583	13.7358	13.5133
163	2.36211	2.25001	10.9751	10.7642	13.7386	13.5174
164	2.36372	2.25213	10.9794	10.7701	13.7413	13.5214
165	2.36531	2.25424	10.9836	10.7759	13.744	13.5253
166	2.36689	2.25633	10.9877	10.7816	13.7466	13.5292
167	2.36845	2.25841	10.9918	10.7872	13.7492	13.5331
168	2.37	2.26046	10.9958	10.7928	13.7518	13.537

169	2.37153	2.26251	10.9998	10.7983	13.7543	13.5408
170	2.37305	2.26453	11.0037	10.8037	13.7568	13.5446
171	2.37455	2.26654	11.0076	10.8091	13.7593	13.5483
172	2.37604	2.26853	11.0114	10.8144	13.7618	13.5521
173	2.37751	2.27051	11.0152	10.8196	13.7642	13.5557
174	2.37897	2.27247	11.0189	10.8248	13.7666	13.5594
175	2.38042	2.27442	11.0226	10.8299	13.7689	13.563
176	2.38185	2.27635	11.0262	10.835	13.7712	13.5666
177	2.38327	2.27826	11.0298	10.84	13.7735	13.5701
178	2.38467	2.28016	11.0333	10.8449	13.7758	13.5737
179	2.38606	2.28205	11.0368	10.8498	13.778	13.5771
180	2.38743	2.28391	11.0402	10.8546	13.7803	13.5806
181	2.3888	2.28577	11.0436	10.8594	13.7824	13.584
182	2.39015	2.28761	11.047	10.8641	13.7846	13.5874
183	2.39148	2.28943	11.0503	10.8688	13.7867	13.5908
184	2.39281	2.29124	11.0536	10.8734	13.7888	13.5941
185	2.39412	2.29304	11.0568	10.8779	13.7909	13.5974
186	2.39542	2.29482	11.06	10.8824	13.793	13.6007
187	2.3967	2.29659	11.0632	10.8869	13.795	13.6039
188	2.39798	2.29834	11.0663	10.8913	13.797	13.6072
189	2.39924	2.30008	11.0694	10.8956	13.799	13.6103
190	2.40049	2.3018	11.0724	10.8999	13.8009	13.6135
191	2.40173	2.30351	11.0754	10.9041	13.8029	13.6166
192	2.40295	2.30521	11.0784	10.9083	13.8048	13.6197
193	2.40417	2.3069	11.0813	10.9125	13.8067	13.6228
194	2.40537	2.30857	11.0842	10.9166	13.8085	13.6258
195	2.40656	2.31022	11.087	10.9207	13.8104	13.6288
196	2.40774	2.31187	11.0898	10.9247	13.8122	13.6318
197	2.40891	2.3135	11.0926	10.9286	13.814	13.6348
198	2.41006	2.31512	11.0954	10.9326	13.8158	13.6377
199	2.41121	2.31672	11.0981	10.9364	13.8175	13.6406
200	2.41234	2.31832	11.1008	10.9403	13.8193	13.6435
201	2.41347	2.31989	11.1034	10.9441	13.821	13.6464
202	2.41458	2.32146	11.106	10.9478	13.8227	13.6492
203	2.41569	2.32302	11.1086	10.9515	13.8244	13.652
204	2.41678	2.32456	11.1112	10.9552	13.826	13.6548
205	2.41786	2.32609	11.1137	10.9588	13.8277	13.6575
206	2.41893	2.32761	11.1162	10.9624	13.8293	13.6603

207	2.42	2.32911	11.1187	10.9659	13.8309	13.663
208	2.42105	2.33061	11.1211	10.9694	13.8325	13.6656
209	2.42209	2.33209	11.1235	10.9729	13.8341	13.6683
210	2.42312	2.33356	11.1259	10.9763	13.8356	13.6709
211	2.42415	2.33502	11.1283	10.9797	13.8372	13.6735
212	2.42516	2.33647	11.1306	10.9831	13.8387	13.6761
213	2.42616	2.3379	11.1329	10.9864	13.8402	13.6787
214	2.42716	2.33933	11.1352	10.9897	13.8417	13.6812
215	2.42814	2.34074	11.1374	10.9929	13.8431	13.6837
216	2.42912	2.34214	11.1396	10.9961	13.8446	13.6862
217	2.43008	2.34354	11.1418	10.9993	13.846	13.6887
218	2.43104	2.34492	11.144	11.0025	13.8475	13.6911
219	2.43199	2.34629	11.1461	11.0056	13.8489	13.6935
220	2.43293	2.34764	11.1483	11.0086	13.8503	13.6959
221	2.43386	2.34899	11.1503	11.0117	13.8516	13.6983
222	2.43479	2.35033	11.1524	11.0147	13.853	13.7007
223	2.4357	2.35166	11.1545	11.0177	13.8543	13.703
224	2.43661	2.35297	11.1565	11.0206	13.8557	13.7053
225	2.43751	2.35428	11.1585	11.0235	13.857	13.7076
226	2.43839	2.35558	11.1605	11.0264	13.8583	13.7099
227	2.43928	2.35686	11.1624	11.0293	13.8596	13.7122
228	2.44015	2.35814	11.1644	11.0321	13.8609	13.7144
229	2.44102	2.35941	11.1663	11.0349	13.8621	13.7166
230	2.44187	2.36066	11.1682	11.0377	13.8634	13.7188
231	2.44272	2.36191	11.17	11.0404	13.8646	13.721
232	2.44356	2.36314	11.1719	11.0431	13.8659	13.7231
233	2.4444	2.36437	11.1737	11.0458	13.8671	13.7253
234	2.44523	2.36559	11.1755	11.0485	13.8683	13.7274
235	2.44605	2.3668	11.1773	11.0511	13.8695	13.7295
236	2.44686	2.368	11.1791	11.0537	13.8706	13.7316
237	2.44766	2.36919	11.1809	11.0563	13.8718	13.7336
238	2.44846	2.37037	11.1826	11.0588	13.873	13.7357
239	2.44925	2.37154	11.1843	11.0613	13.8741	13.7377
240	2.45003	2.3727	11.186	11.0638	13.8752	13.7397
241	2.45081	2.37385	11.1877	11.0663	13.8764	13.7417
242	2.45158	2.375	11.1893	11.0687	13.8775	13.7437
243	2.45234	2.37613	11.191	11.0712	13.8786	13.7456
244	2.4531	2.37726	11.1926	11.0735	13.8796	13.7476

245	2.45385	2.37838	11.1942	11.0759	13.8807	13.7495
246	2.45459	2.37949	11.1958	11.0783	13.8818	13.7514
247	2.45533	2.38059	11.1974	11.0806	13.8828	13.7533
248	2.45606	2.38168	11.1989	11.0829	13.8839	13.7551
249	2.45678	2.38277	11.2005	11.0852	13.8849	13.757
250	2.45749	2.38384	11.202	11.0874	13.886	13.7588
251	2.45821	2.38491	11.2035	11.0897	13.887	13.7607
252	2.45891	2.38597	11.205	11.0919	13.888	13.7625
253	2.45961	2.38702	11.2065	11.0941	13.889	13.7643
254	2.4603	2.38807	11.2079	11.0962	13.89	13.766
255	2.46099	2.3891	11.2094	11.0984	13.8909	13.7678
256	2.46167	2.39013	11.2108	11.1005	13.8919	13.7695
257	2.46234	2.39115	11.2122	11.1026	13.8929	13.7713
258	2.46301	2.39216	11.2136	11.1047	13.8938	13.773
259	2.46367	2.39317	11.215	11.1068	13.8948	13.7747
260	2.46433	2.39417	11.2164	11.1088	13.8957	13.7764
261	2.46498	2.39516	11.2178	11.1108	13.8966	13.778
262	2.46562	2.39614	11.2191	11.1128	13.8975	13.7797
263	2.46626	2.39711	11.2204	11.1148	13.8984	13.7813
264	2.4669	2.39808	11.2218	11.1168	13.8993	13.783
265	2.46753	2.39904	11.2231	11.1187	13.9002	13.7846
266	2.46815	2.39999	11.2244	11.1207	13.9011	13.7862
267	2.46877	2.40094	11.2256	11.1226	13.902	13.7878
268	2.46938	2.40188	11.2269	11.1245	13.9029	13.7893
269	2.46999	2.40281	11.2282	11.1263	13.9037	13.7909
270	2.47059	2.40374	11.2294	11.1282	13.9046	13.7924
271	2.47119	2.40465	11.2306	11.13	13.9054	13.794
272	2.47178	2.40557	11.2319	11.1319	13.9063	13.7955
273	2.47237	2.40647	11.2331	11.1337	13.9071	13.797
274	2.47295	2.40737	11.2343	11.1354	13.9079	13.7985
275	2.47353	2.40826	11.2355	11.1372	13.9087	13.8
276	2.47411	2.40914	11.2366	11.139	13.9095	13.8014
277	2.47467	2.41002	11.2378	11.1407	13.9103	13.8029
278	2.47524	2.41089	11.2389	11.1424	13.9111	13.8044
279	2.4758	2.41176	11.2401	11.1441	13.9119	13.8058
280	2.47635	2.41262	11.2412	11.1458	13.9127	13.8072
281	2.4769	2.41347	11.2423	11.1475	13.9135	13.8086
282	2.47745	2.41432	11.2434	11.1492	13.9142	13.81

283	2.47799	2.41516	11.2445	11.1508	13.915	13.8114
284	2.47852	2.41599	11.2456	11.1525	13.9158	13.8128
285	2.47906	2.41682	11.2467	11.1541	13.9165	13.8141
286	2.47958	2.41764	11.2478	11.1557	13.9172	13.8155
287	2.48011	2.41845	11.2488	11.1573	13.918	13.8168
288	2.48063	2.41926	11.2499	11.1588	13.9187	13.8182
289	2.48114	2.42007	11.2509	11.1604	13.9194	13.8195
290	2.48165	2.42087	11.2519	11.1619	13.9201	13.8208
291	2.48216	2.42166	11.2529	11.1635	13.9209	13.8221
292	2.48266	2.42244	11.2539	11.165	13.9216	13.8234
293	2.48316	2.42323	11.2549	11.1665	13.9223	13.8247
294	2.48365	2.424	11.2559	11.168	13.923	13.8259
295	2.48414	2.42477	11.2569	11.1695	13.9236	13.8272
296	2.48463	2.42553	11.2579	11.1709	13.9243	13.8284
297	2.48511	2.42629	11.2588	11.1724	13.925	13.8297
298	2.48559	2.42705	11.2598	11.1738	13.9257	13.8309
299	2.48606	2.42779	11.2607	11.1752	13.9263	13.8321
300	2.48654	2.42854	11.2617	11.1766	13.927	13.8333

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**Table S10.** Calculated CASSCF Ms ( $N\mu_B$ ) vs. H (T) data for all the complexes at 2K.

H (T)	Ms ( $N\mu_B$ )					
	1a	1b	2a	2b	3a	3b
0.0	0.00017	0.00015	0.00071	0.00061	0.00106	0.0011
0.1	0.16547	0.14812	0.70172	0.60163	1.03951	1.07718
0.2	0.32772	0.29375	1.34964	1.16414	1.96201	2.02849
0.3	0.48381	0.4346	1.90789	1.65971	2.70466	2.78807
0.4	0.63134	0.56873	2.36439	2.07642	3.26477	3.35543
0.5	0.76855	0.69466	2.72515	2.41567	3.67266	3.76454
0.6	0.89441	0.81143	3.00505	2.68662	3.96604	4.05599
0.7	1.00847	0.91853	3.22088	2.90119	4.17759	4.2642
0.8	1.11086	1.01588	3.3877	3.07104	4.33191	4.41469
0.9	1.20207	1.10372	3.51773	3.20621	4.4464	4.52529
1.0	1.28283	1.18251	3.62035	3.31479	4.533	4.60811
1.1	1.35405	1.25288	3.70252	3.40307	4.59986	4.67136
1.2	1.41667	1.31553	3.76939	3.47582	4.65255	4.72061
1.3	1.47165	1.37121	3.8247	3.53666	4.6949	4.75966
1.4	1.5199	1.42062	3.87122	3.58827	4.72957	4.79117
1.5	1.56224	1.46448	3.91096	3.6327	4.75847	4.81701
1.6	1.59943	1.50341	3.94543	3.67147	4.78295	4.8385
1.7	1.63216	1.53801	3.97576	3.70576	4.80398	4.85662
1.8	1.661	1.5688	4.00279	3.73645	4.82232	4.87208
1.9	1.68649	1.59625	4.02717	3.76422	4.83849	4.88543
2.0	1.70907	1.62077	4.0494	3.78962	4.85292	4.89707
2.1	1.72912	1.64272	4.06986	3.81305	4.86594	4.90732
2.2	1.74699	1.66244	4.08886	3.83485	4.87778	4.91641
2.3	1.76296	1.68018	4.10665	3.85528	4.88865	4.92456
2.4	1.77728	1.69619	4.12341	3.87456	4.89871	4.9319
2.5	1.79016	1.71068	4.1393	3.89284	4.90807	4.93857
2.6	1.80178	1.72384	4.15445	3.91028	4.91686	4.94466
2.7	1.81231	1.73581	4.16897	3.92699	4.92514	4.95026
2.8	1.82187	1.74674	4.18293	3.94306	4.93299	4.95544
2.9	1.83057	1.75675	4.19642	3.95858	4.94046	4.96026
3.0	1.83853	1.76594	4.20948	3.97361	4.94761	4.96476
3.1	1.84583	1.7744	4.22218	3.9882	4.95448	4.96899
3.2	1.85255	1.78221	4.23455	4.00241	4.9611	4.97297
3.3	1.85874	1.78944	4.24664	4.01627	4.96749	4.97675
3.4	1.86447	1.79614	4.25846	4.02982	4.97369	4.98033

3.5	1.86978	1.80238	4.27006	4.0431	4.97971	4.98376
3.6	1.87472	1.8082	4.28144	4.05612	4.98558	4.98703
3.7	1.87933	1.81364	4.29264	4.06892	4.99131	4.99018
3.8	1.88365	1.81874	4.30367	4.0815	4.99691	4.99321
3.9	1.88769	1.82353	4.31454	4.0939	5.0024	4.99614
4.0	1.89148	1.82803	4.32528	4.10612	5.00778	4.99897
4.1	1.89506	1.83228	4.33588	4.11817	5.01308	5.00172
4.2	1.89844	1.83629	4.34636	4.13008	5.01829	5.0044
4.3	1.90163	1.84009	4.35673	4.14184	5.02342	5.00701
4.4	1.90466	1.8437	4.36701	4.15348	5.02848	5.00956
4.5	1.90754	1.84712	4.37718	4.165	5.03347	5.01205
4.6	1.91027	1.85038	4.38728	4.1764	5.03841	5.01449
4.7	1.91289	1.85349	4.39729	4.1877	5.04329	5.01689
4.8	1.91538	1.85645	4.40722	4.1989	5.04812	5.01924
4.9	1.91777	1.85929	4.41709	4.21001	5.0529	5.02156
5.0	1.92005	1.86201	4.42689	4.22103	5.05764	5.02384

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