# Supporting Information

# Breaking the Axiality of Pentagonal-Bipyramidal Dysprosium(III) Single-Molecule Magnets with Pyrazolate

## Ligands

Zi-Han Li,<sup>a</sup> Yuan-Qi Zhai,<sup>a</sup> Wei-Peng Chen,<sup>a</sup> Qian-Cheng Luo,<sup>a</sup> Tian Han<sup>a</sup> and Yan-Zhen Zheng<sup>\*a</sup>

<sup>a</sup>Frontier Institute of Science and Technology (FIST), School of Chemistry, Xi'an Jiaotong University Shenzhen Research School, State Key Laboratory of Mechanical Behaviour for Materials, MOE Key Laboratory for Nonequilibrium Synthesis of Condensed Matter, Xi'an Key Laboratory of Sustainable Energy and Materials Chemistry, Xi'an Jiaotong University, 99 Yanxiang Road, Xi'an, Shaanxi 710054, P. R. China. E-mail: zheng.yanzhen@xjtu.edu.cn

#### (2) 100 (1) 100 (3)Transmissivity / % % Transmissivity / % Transmissivity / 75 50 1500 2500 2000 3000 2500 2000 1500 1000 4000 3500 3000 1000 3500 3000 2500 2000 1500 4000 3500 4000 1000 Wavenumbers / cm Wavenumbers / cm<sup>-1</sup> Wavenumbers / cm (6) 100-(4) 100 (5) 100 Transmissivity / % Transmissivity / % %/ Transmissivity 75 75 50 50 3500 1500 1000 4000 3000 2500 2000 3000 2500 3000 2500 4000 3500 2000 1500 1000 4000 3500 2000 1500 1000 Wavenumbers / cm Wavenumbers / cm-Wavenumbers / cm<sup>-1</sup>

#### 1. Infrared spectrum

Figure S1. Infrared spectra of complexes 1 - 6.



Figure S2. Infrared spectra of complexes 7 - 10.

### 2. X-ray Crystallography Data

Table S1. Selected bond lengths (Å) and angles (deg) for complex 1.

Dy(1)-N(1)	2.346(3)	Dy(1)-N(2)	2.426(4)
Dy(1)-cen(N-N)	2.303(5)	Dy(1)-O(1)	2.382(3)
Dy(1)-O(2)	2.431(3)	Dy(1)-O(3)	2.441(3)
Dy(1)-O(4)	2.385(3)	Dy(1)-O(5)	2.461(3)
Dy(1)-Cl(1)	2.6082(10)	O(1)-Dy(1)-O(2)	71.27(9)
O(2)-Dy(1)-O(3)	72.59(3)	O(3)-Dy(1)-O(4)	72.80(9)
O(4)-Dy(1)-O(5)	72.01(9)	O(5)-Dy(1)-O(1)	71.96(10)
cen(N-N)-Dy(1)-Cl(1)	175.80(2)		

Table S2. Selected bond lengths (Å) and angles (deg) for complex 2.

Dy(1)-N(1)	2.364(4)	Dy(1)-N(2)	2.317(4)
Dy(1)-cen(N-N)	2.235(5)	Dy(1)-O(1)	2.458(3)
Dy(1)-O(2)	2.390(3)	Dy(1)-O(3)	2.448(3)
Dy(1)-O(4)	2.437(3)	Dy(1)-O(5)	2.457(3)
Dy(1)-Cl(1)	2.6216(13)	O(1)-Dy(1)-O(2)	72.39(12)
O(2)-Dy(1)-O(3)	73.13(12)	O(3)-Dy(1)-O(4)	72.37(11)
O(4)-Dy(1)-O(5)	71.79(10)	O(5)-Dy(1)-O(1)	70.44(10)
cen(N-N)-Dy(1)-Cl(1)	176.53(2)		
Table S3. Selected bond leng	gths (Å) and angles (d	leg) for complex <b>3</b> .	
Dy(1)-N(1)	2.320(3)	Dy(1)-N(2)	2.353(3)
Dy(1)-cen(N-N)	2.232(3)	Dy(1)-O(1)	2.410(3)
Dy(1)-O(2)	2.478(2)	Dy(1)-O(3)	2.402(2)
Dy(1)-O(4)	2.464(2)	Dy(1)-O(5)	2.446(3)
Dy(1)-Cl(1)	2.6184(10)	O(1)-Dy(1)-O(2)	71.87(9)
O(2)-Dy(1)-O(3)	72.48(9)	O(3)-Dy(1)-O(4)	71.00(9)
O(4)-Dy(1)-O(5)	72.51(9)	O(5)-Dy(1)-O(1)	71.87(9)
cen(N-N)-Dy(1)-Cl(1)	177.44(3)		

Table S4. Selected bond lengths (Å) and angles (deg) for complex 4.

Dy(1)-N(1)	2.331(7)	Dy(1)-N(2)	2.344(6)
Dy(1)-cen(N-N)	2.233(5)	Dy(1)-O(1)	2.427(6)
Dy(1)-O(2)	2.465(6)	Dy(1)-O(3)	2.452(6)
Dy(1)-O(4)	2.420(6)	Dy(1)-O(5)	2.493(6)
Dy(1)-Cl(1)	2.623(2)	O(1)-Dy(1)-O(2)	72.2 (2)
O(2)-Dy(1)-O(3)	72.3(2)	O(3)-Dy(1)-O(4)	71.1(2)
O(4)-Dy(1)-O(5)	73.3 (2)	O(5)-Dy(1)-O(1)	72.9(2)
cen(N-N)-Dy(1)-Cl(1)	177.94(6)		

Table S5. Selected bond lengths (Å) and angles (deg) for complex 5.

Dy(1)-N(1)	2.348(5)	Dy(1)-N(2)	2.334(5)
Dy(1)-cen(N-N)	2.238(5)	Dy(1)-O(1)	2.438(4)
Dy(1)-O(2)	2.428(4)	Dy(1)-O(3)	2.476(4)
Dy(1)-O(4)	2.417(4)	Dy(1)-O(5)	2.474(4)
Dy(1)-Cl(1)	2.6122(15)	O(1)-Dy(1)-O(2)	70.31(13)
O(2)-Dy(1)-O(3)	73.44(13)	O(3)-Dy(1)-O(4)	74.91(13)
O(4)-Dy(1)-O(5)	71.51(13)	O(5)-Dy(1)-O(1)	72.75(13)
cen(N-N)-Dy(1)-Cl(1)	175.94(5)		

Table S6. Selected bond lengths  $(\text{\AA})$  and angles (deg) for complex 6.

Dy(1)-N(1)2.347(5) $Dy(1)-N(2)$ 2.333(5) $Dy(1)-cen(N-N)$ 2.242(5) $Dy(1)-O(1)$ 2.406(4) $Dy(1)-O(2)$ 2.464(4) $Dy(1)-O(3)$ 2.445(4) $Dy(1)-O(4)$ 2.435(4) $Dy(1)-O(5)$ 2.467 (4) $Dy(1)-Cl(1)$ 2.6194(18) $O(1)-Dy(1)-O(2)$ 71.96(15) $O(2)-Dy(1)-O(3)$ 71.38(14) $O(3)-Dy(1)-O(4)$ 71.04(14) $O(4)-Dy(1)-O(5)$ 72.57(15) $O(5)-Dy(1)-O(1)$ 73.17(16)		8 (	-8/ F		
Dy(1)-cen(N-N)       2.242(5)       Dy(1)-O(1)       2.406(4)         Dy(1)-O(2)       2.464(4)       Dy(1)-O(3)       2.445(4)         Dy(1)-O(4)       2.435(4)       Dy(1)-O(5)       2.467 (4)         Dy(1)-Cl(1)       2.6194(18)       O(1)-Dy(1)-O(2)       71.96(15)         O(2)-Dy(1)-O(3)       71.38(14)       O(3)-Dy(1)-O(4)       71.04(14)         O(4)-Dy(1)-O(5)       72.57(15)       O(5)-Dy(1)-O(1)       73.17(16)	Dy(1)-N(1)	2.347(5)	Dy(1)-N(2)	2.333(5)	
Dy(1)-O(2)       2.464(4)       Dy(1)-O(3)       2.445(4)         Dy(1)-O(4)       2.435(4)       Dy(1)-O(5)       2.467 (4)         Dy(1)-Cl(1)       2.6194(18)       O(1)-Dy(1)-O(2)       71.96(15)         O(2)-Dy(1)-O(3)       71.38(14)       O(3)-Dy(1)-O(4)       71.04(14)         O(4)-Dy(1)-O(5)       72.57(15)       O(5)-Dy(1)-O(1)       73.17(16)	Dy(1)-cen(N-N)	2.242(5)	Dy(1)-O(1)	2.406(4)	
Dy(1)-O(4)       2.435(4)       Dy(1)-O(5)       2.467 (4)         Dy(1)-Cl(1)       2.6194(18)       O(1)-Dy(1)-O(2)       71.96(15)         O(2)-Dy(1)-O(3)       71.38(14)       O(3)-Dy(1)-O(4)       71.04(14)         O(4)-Dy(1)-O(5)       72.57(15)       O(5)-Dy(1)-O(1)       73.17(16)	Dy(1)-O(2)	2.464(4)	Dy(1)-O(3)	2.445(4)	
Dy(1)-Cl(1)       2.6194(18)       O(1)-Dy(1)-O(2)       71.96(15)         O(2)-Dy(1)-O(3)       71.38(14)       O(3)-Dy(1)-O(4)       71.04(14)         O(4)-Dy(1)-O(5)       72.57(15)       O(5)-Dy(1)-O(1)       73.17(16)         cen(N-N)-Dy(1)-Cl(1)       176.52(5)       Image: Control of the second se	Dy(1)-O(4)	2.435(4)	Dy(1)-O(5)	2.467 (4)	
O(2)-Dy(1)-O(3)       71.38(14)       O(3)-Dy(1)-O(4)       71.04(14)         O(4)-Dy(1)-O(5)       72.57(15)       O(5)-Dy(1)-O(1)       73.17(16)         cen(N-N)-Dy(1)-Cl(1)       176.52(5)	Dy(1)-Cl(1)	2.6194(18)	O(1)-Dy(1)-O(2)	71.96(15)	
O(4)-Dy(1)-O(5) 72.57(15) O(5)-Dy(1)-O(1) 73.17(16)	O(2)-Dy(1)-O(3)	71.38(14)	O(3)-Dy(1)-O(4)	71.04(14)	
cen(N-N)-Dv(1)-Cl(1) 176 52(5)	O(4)-Dy(1)-O(5)	72.57(15)	O(5)-Dy(1)-O(1)	73.17(16)	
	cen(N-N)-Dy(1)-Cl(1)	176.52(5)			

Table S7. Selected bond lengths  $(\text{\AA})$  and angles (deg) for complex 7.

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Dy(1)-N(1)	2.4505(18)	Dy(1)-N(2)	2.3553(19)	
Dy(1)-N(3)	2.4505(18)	Dy(1)-N(4)	2.3553(19)	
Dy(1)-cen(N-N)	2.306(5)	Dy(1)-O(1)	2.4508(15)	
Dy(1)-O(2)	2.4213(15)	Dy(1)-O(3)	2.531(2)	
Dy(1)-O(4)	2.4508(15)	Dy(1)-O(5)	2.4213(15)	
O(1)-Dy(1)-O(2)	72.92(5)	O(2)-Dy(1)-O(3)	72.23(3)	
O(3)-Dy(1)-O(4)	72.23(3)	O(4)-Dy(1)-O(5)	72.92(5)	
O(5)-Dy(1)-O(1)	73.06(7)	cen(N-N)-Dy(1)- cen(N-N)	178.71(9)	
				_

Table S8. Selected bond lengths (Å) and angles (deg) for complex  ${\bf 8}.$ 

Dy(1)-N(1)	2.370(6)	Dy(1)-N(2)	2.396(6)
Dy(1)-N(3)	2.382(8)	Dy(1)-N(4)	2.353(8)
Dy(1)-cen(N-N)(1)	2.296(8)	Dy(1)-cen(N-N)(2)	2.270(8)
Dy(1)-O(1)	2.470(6)	Dy(1)-O(2)	2.499(5)
Dy(1)-O(3)	2.451(4)	Dy(1)-O(4)	2.472(6)
Dy(1)-O(5)	2.462(7)	O(1)-Dy(1)-O(2)	71.4(2)
O(2)-Dy(1)-O(3)	72.4(2)	O(3)-Dy(1)-O(4)	75.5(2)
O(4)-Dy(1)-O(5)	70.7(2)	O(5)-Dy(1)-O(1)	71.81(17)
cen(N-N)-Dy(1)-cen(N-N)	174.23(27)	cen(N-N)-Dy(1)-N(5)	83.39(3)
cen(N-N)-Dy(1)-N(5)	95.50(4)	cen(N-N)-Dy(1)-N(5)	91.93(3)
cen(N-N)-Dy(1)-N(5)	84.57(2)	cen(N-N)-Dy(1)-N(5)	92.14(5)

Table S9. Selected bond lengths (Å) and angles (deg) for complex 9.

Dy(1)-N(1)	2.407(3)	Dy(1)-N(2)	2.397(3)
Dy(1)-N(3)	2.364(3)	Dy(1)-N(4)	2.394(3)
Dy(1)-cen(N-N)(1)	2.301(6)	Dy(1)-cen(N-N)(2)	2.278(6)
Dy(1)-N(5)	2.567(3)	Dy(1)-N(6)	2.626(3)
Dy(1)-N(7)	2.534(3)	Dy(1)-N(8)	2.628(3)
Dy(1)-N(9)	2.578(3)	N(5)-Dy(1)-N(6)	70.71(10)
N(6)-Dy(1)-N(7)	76.52(10)	N(7)-Dy(1)-N(8)	72.93(10)
N(8)-Dy(1)-N(9)	69.77(10)	N(9)-Dy(1)-N(5)	73.27(10)
cen(N-N)-Dy(1)-cen(N-N)	177.66(22)	cen(N-N)-Dy(1)-N(5)	87.71(3)
cen(N-N)-Dy(1)-N(6)	89.50(5)	cen(N-N)-Dy(1)-N(7)	95.79(6)
cen(N-N)-Dy(1)-N(8)	81.00(3)	cen(N-N)-Dy(1)-N(9)	96.48(7)

Table S10. Selected bond lengths (Å) and angles (deg) for complex  $10. \label{eq:stable}$ 

Dy(1)-N(1)	2.384(5)	Dy(1)-N(2)	2.401(4)
Dy(1)-N(3)	2.434(4)	Dy(1)-N(4)	2.383(4)
Dy(1)-cen(N-N)(1)	2.291(16)	Dy(1)-cen(N-N)(2)	2.309(16)
Dy(1)-N(5)	2.549(5)	Dy(1)-N(6)	2.564(4)
Dy(1)-N(7)	2.576(4)	Dy(1)-N(8)	2.577(4)
Dy(1)-N(9)	2.577(5)	N(5)-Dy(1)-N(6)	75.62(14)
N(6)-Dy(1)-N(7)	69.58(14)	N(7)-Dy(1)-N(8)	71.10(14)
N(8)-Dy(1)-N(9)	70.72(13)	N(9)-Dy(1)-N(5)	78.29(14)
cen(N-N)-Dy(1)-cen(N-N)	175.16(37)	cen(N-N)-Dy(1)-N(5)	78.58(3)
cen(N-N)-Dy(1)-N(6)	96.94(4)	cen(N-N)-Dy(1)-N(7)	81.03(5)
cen(N-N)-Dy(1)-N(8)	94.86(4)	cen(N-N)-Dy(1)-N(9)	96.11(5)

Complex	1	2	3	4
Empirical formula	C <sub>52</sub> H <sub>70</sub> BClDyF <sub>3</sub> N <sub>2</sub> O <sub>6</sub>	C48H65BClDyN2O5	C54H69BClDyN2O6	C53H77BClDyN2O7
Formula weight / g mol <sup>-1</sup>	1084.86	958.78	1050.87	1062.92
Temperature / K	150	150	150	150
Crystal system	monoclinic	monoclinic	triclinic	monoclinic
Space group	$P2_{1}/c$	C2/c	$P\overline{1}$	<i>C</i> 2/ <i>c</i>
<i>a</i> / Å	12.972(2)	19.719(8)	12.130(3)	17.416(6)
<i>b</i> / Å	23.064(4)	16.286(7)	12.685(3)	19.019(6)
<i>c</i> / Å	17.494(3)	28.674(12)	17.772(4)	33.756(13)
α/°	90	90	81.348(3)	90
eta / °	104.213(2)	93.945(5)	77.247(3)	93.763(3)
γ / °	90	90	85.637(3)	90
$V/  m \AA^3$	5073.7(15)	9186(6)	2634.2(11)	11157(7)
Ζ	4	8	2	8
$ ho_{ m calc}$ / g cm <sup>-3</sup>	1.420	1.384	1.325	1.266
F(000)	2236.0	3944.0	1086.0	4424.0
Crystal size/ mm <sup>3</sup>	0.18×0.16×0.15	0.26 ×0.17×0.15	0.14×0.15×0.13	0.24×0.18×0.13
Radiation	ΜοΚα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	ΜοΚα (λ = 0.71073)
2 heta range / °	2.98 to 55.35	2.848 to 53.134	3.25 to 53.486	3.174 to 49.998
Reflections collected	54309	36222	28634	47832
Goodness-of-fit on $F^2$	1.105	1.103	1.026	1.172
<i>R</i> indexes [I>= $2\sigma$	$R_1 = 0.0390, wR_2 =$	$R_1 = 0.0406, wR_2$	$R_1 = 0.0375, wR_2 =$	$R_1 = 0.0723, wR_2 =$
(I)]	0.0883	=0.0933	0.0936	0.1854
Final <i>R</i> indexes [all data]	$R_1 = 0.0551, wR_2 = 0.0977$	$R_1 = 0.0566, wR_2 = 0.1001$	$R_1 = 0.0449, wR_2 = 0.0987$	$R_1 = 0.0890, wR_2 = 0.1949$

 Table S11. X-ray crystallographic data for complexes 1 - 4.

Complex	5	6	7
Empirical formula	C57H85BClDyN2O7	$C_{51}H_{73}BClDyN_2O_7$	$C_{52}H_{64}BDyF_6N_4O_5$
Formula weight / g mol-1	1119.03	1034.87	1112.38
Temperature / K	150	150	150
Crystal system	triclinic	triclinic	monoclinic
Space group	$P\overline{1}$	$P\overline{1}$	C2/c
a / Å	12.661(3)	12.861(6)	10.539(3)
b / Å	12.944(3)	13.033(6)	30.137(9)
<i>c</i> / Å	18.009(4)	16.666(8)	15.602(5)
lpha / °	75.837(3)	77.974(6)	90
eta / °	86.900(3)	78.722(6)	96.835(4)
γ / °	82.869(3)	80.447(6)	90
V / Å <sup>3</sup>	2838.7(11)	2657(2)	4920(3)
Ζ	2	2	4
$ ho_{ m calc}$ / g cm <sup>-3</sup>	1.307	1.287	1.502
F(000)	1166.0	1064.0	2276.0
Crystal size/ mm <sup>3</sup>	0.22×0.19×0.17	0.15 ×0.14×0.12	0.3×0.26×0.24
Radiation	MoKa ( $\lambda = 0.71073$ )	MoK $\alpha$ ( $\lambda = 0.71073$ )	MoK $\alpha$ ( $\lambda = 0.71073$ )
2 heta range / °	2.332 to 53.434	3.222 to 52.842	3.77 to 55.142
Reflections collected	29433	27616	28194
Goodness-of-fit on $F^2$	1.038	1.036	1.085
<i>R</i> indexes [I>= $2\sigma$ (I)]	$R_1 = 0.0533, wR_2 = 0.1406$	$R_1 = 0.0506, wR_2$ =0.1366	$R_1 = 0.0233, wR_2 = 0.0578$
Final <i>R</i> indexes [all data]	$R_1 = 0.0784, wR_2 = 0.1577$	$R_1 = 0.0741, wR_2 = 0.1541$	$R_1 = 0.0262, wR_2 = 0.0594$

 Table S12. X-ray crystallographic data for complexes 5 - 7.

Complex	8	9	10
Empirical formula	$C_{50}H_{66}BDyN_4O_5$	$C_{62}H_{58}BDyN_{11}$	$C_{45}H_{41}BDyN_9S_5$
Formula weight / g mol <sup>-1</sup>	976.37	1130.50	1041.48
Temperature / K	150	150	150
Crystal system	orthorhombic	monoclinic	orthorhombic
Space group	P212121	$P2_{1}/n$	Pbca
<i>a</i> / Å	10.841(4)	9.619(3)	19.857(14)
b / Å	13.215 (5)	30.938(8)	19.247(14)
<i>c</i> / Å	33.326(13)	18.634(5)	23.965(17)
α/°	90	90	90
eta / °	90	94.845(4)	90
γ / °	90	90	90
V / Å <sup>3</sup>	4774(3)	5526(3)	9159(11)
Ζ	4	4	8
$ ho_{ m calc}$ / g cm <sup>-3</sup>	1.358	1.359	1.511
F(000)	2020.0	2312.0	4200.0
Crystal size/ mm <sup>3</sup>	0.32×0.25×0.19	0.32×0.16×0.15	0.66×0.54×0.48
Radiation	MoK $\alpha$ ( $\lambda = 0.71073$ )	MoK $\alpha$ ( $\lambda = 0.71073$ )	MoKa ( $\lambda = 0.71073$ )
2 heta range / °	3.316 to 52.116	3.426 to 52.928	3.398 to 53.108
Reflections collected	45410	33129	70169
Goodness-of-fit on $F^2$	1.016	1.035	1.150
<i>R</i> indexes [I>= $2\sigma$ (I)]	$R_1 = 0.0387, wR_2 = 0.0865$	$R_1 = 0.0387, wR_2 = 0.0865$	$R_1 = 0.0440, wR_2 = 0.1031$
Final <i>R</i> indexes [all data]	$R_1 = 0.0506, wR_2 = 0.0918$	$R_1 = 0.0506, wR_2 = 0.0918$	$R_1 = 0.0649, wR_2 = 0.1148$

 Table S13. X-ray crystallographic data for complexes 8 - 10.



**Figure S3**. Molecular packing arrangement of **1**; dashed line shows the nearest intermolecular Dy...Dy separation (Å). Hydrogen atoms and solvent molecules are omitted for clarity. Color codes: Dy, orange; O, red; N, blue; Cl, green; F, light green; B, light orange; C, grey.



**Figure S4.** Molecular packing arrangement of **2**; dashed line shows the nearest intermolecular Dy...Dy separation (Å). Hydrogen atoms and solvent molecules are omitted for clarity. Color codes: Dy, orange; O, red; N, blue; Cl, green; F, light green; B, light orange; C, grey.



**Figure S5.** Molecular packing arrangement of **3**; dashed line shows the nearest intermolecular Dy...Dy separation (Å). Hydrogen atoms and solvent molecules are omitted for clarity. Color codes: Dy, orange; O, red; N, blue; Cl, green; F, light green; B, light orange; C, grey.



**Figure S6**. Molecular packing arrangement of **4**; dashed line shows the nearest intermolecular Dy...Dy separation (Å). Hydrogen atoms and solvent molecules are omitted for clarity. Color codes: Dy, orange; O, red; N, blue; Cl, green; B, light orange; C, grey.



**Figure S7**. Molecular packing arrangement of **5**; dashed line shows the nearest intermolecular Dy…Dy separation (Å). Hydrogen atoms and solvent molecules are omitted for clarity. Color codes: Dy, orange; O, red; N, blue; Cl, green; B, light orange; C, grey.



**Figure S8**. Molecular packing arrangement of **6**; dashed line shows the nearest intermolecular Dy…Dy separation (Å). Hydrogen atoms and solvent molecules are omitted for clarity. Color codes: Dy, orange; O, red; N, blue; Cl, green; B, light orange; C, grey.



**Figure S9**. Molecular packing arrangement of **7**; dashed line shows the nearest intermolecular Dy...Dy separation (Å). Hydrogen atoms and solvent molecules are omitted for clarity. Color codes: Dy, orange; O, red; N, blue; Cl, green; F, light green; B, light orange; C, grey.



**Figure S10**. Molecular packing arrangement of **8**; dashed line shows the nearest intermolecular Dy…Dy separation (Å). Hydrogen atoms and solvent molecules are omitted for clarity. Color codes: Dy, orange; O, red; N, blue; Cl, green; F, light green; B, light orange; C, grey.



**Figure S11**. Molecular packing arrangement of **9**; dashed line shows the nearest intermolecular Dy…Dy separation (Å). Hydrogen atoms and solvent molecules are omitted for clarity. Color codes: Dy, orange; O, red; N, blue; Cl, green; F, light green; B, light orange; C, grey.



**Figure S12**. Molecular packing arrangement of **10**; dashed line shows the nearest intermolecular Dy...Dy separation (Å). Hydrogen atoms and solvent molecules are omitted for clarity. Color codes: Dy, orange; O, red; N, blue; Cl, green; F, light green; B, light orange; C, grey.

#### 3. Magnetic Property



Figure S13. Temperature-dependent dc magnetic susceptibility (measured under 1000 Oe) for 1 - 6.



Figure S14. Temperature-dependent dc magnetic susceptibility (measured under 1000 Oe) for 7 - 10.



Figure S15. Field dependent magnetization for 1 - 6.



Figure S16. Field dependent magnetization for 7 - 10.



**Figure S17.** Variable-temperature in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **1**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S18.** Variable-temperature in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **2**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S19.** Variable-temperature in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **3**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S20.** Variable-temperature in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **4**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S21.** Variable-temperature in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **5**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S22.** Variable-temperature in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **6**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S23.** Variable-temperature in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **7**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S24.** Variable-temperature in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **8**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S25.** Variable-temperature in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **9**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S26.** Variable-temperature in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **10**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S27.** Variable frequency in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **1**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S28.** Variable frequency in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **2**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S29.** Variable frequency in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **3**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S30.** Variable frequency in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **4**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S31.** Variable frequency in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **5**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S32.** Variable frequency in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **6**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S33.** Variable frequency in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **7**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S34.** Variable frequency in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **9**, in zero static field and an oscillating field of 3.5 Oe.



**Figure S35.** Variable frequency in-phase (top) and out-of-phase (bottom) magnetic susceptibility of **10**, in zero static field and an oscillating field of 3.5 Oe.

![](_page_26_Figure_0.jpeg)

**Figure S36.** Cole–Cole plots for **1** collected from 2 K to 11 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_26_Figure_2.jpeg)

**Figure S37.** Cole–Cole plots for **2**collected from 2 K to 17 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_27_Figure_0.jpeg)

**Figure S38.** Cole–Cole plots for **3** collected from 2 K to 23 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_27_Figure_2.jpeg)

**Figure S39.** Cole–Cole plots for **4** collected from 2 K to 25 K. Lines represent fits with a generalized Debye model used to extract relaxation times..

![](_page_28_Figure_0.jpeg)

**Figure S40.** Cole–Cole plots for **5** collected from 2 K to 25 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_28_Figure_2.jpeg)

**Figure S41.** Cole–Cole plots for **6** collected from 2 K to 35 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_29_Figure_0.jpeg)

**Figure S42.** Cole–Cole plots for **7** collected from 2 K to 28 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_29_Figure_2.jpeg)

**Figure S43.** Cole–Cole plots for **8** collected from 2 K to 35 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_30_Figure_0.jpeg)

**Figure S44.** Cole–Cole plots for **9** collected from 2 K to 8 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_30_Figure_2.jpeg)

**Figure S45.** Cole–Cole plots for **9** collected from 10 K to 18 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_31_Figure_0.jpeg)

**Figure S46.** Cole–Cole plots for **9** collected from 20 K to 32 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_31_Figure_2.jpeg)

**Figure S47.** Cole–Cole plots for **10** collected from 2 K to 12 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_32_Figure_0.jpeg)

**Figure S48.** Cole–Cole plots for **10** collected from 14 K to 29 K. Lines represent fits with a generalized Debye model used to extract relaxation times.

![](_page_32_Figure_2.jpeg)

**Figure S49.** Plots of magnetic susceptibility vs temperature during FC (black) and ZFC (red) measurements for **9**.

![](_page_33_Figure_0.jpeg)

Figure S50. Plots of magnetic susceptibility vs temperature during FC (black) and ZFC (red) measurements for 10.

![](_page_33_Figure_2.jpeg)

**Figure S51.** Magnetic hysteresis loops for **9** between 2 K and 5 K. The data was collected with the field sweeping rate of 12 Oe s<sup>-1</sup>.

![](_page_34_Figure_0.jpeg)

**Figure S52.** Magnetic hysteresis loops for **10** between 2 K and 5 K. The data was collected with the field sweeping rate of 12 Oe  $s^{-1}$ .

#### 4. Electronic Structure Calculations

Energy	Energy	gx	$g_{\mathrm{y}}$	gz	g <sub>z</sub> Angle (°)	Wavefunction
(cm <sup>-1</sup> )	(K)					
0	0	0.02	0.05	19.44		$10\% \pm15/2>+12\% \pm11/2>+18\% \pm9/2>+$
						$18\% \pm7/2>+15\% \pm5/2>+10\% \pm3/2>$
74	106	0.23	0.37	18.53	59	85%  ±15/2>
125	179	0.44	1.51	16.77	90	$29\% \pm13/2>+36\% \pm11/2>+17\% \pm9/2>$
158	227	3.07	4.81	10.33	79	$32\% \pm13/2>+27\% \pm9/2>$
193	277	2.70	3.58	8.94	22	$14\% \pm13/2>+10\% \pm11/2>+21\% \pm7/2>$
237	340	0.56	0.79	13.51	27	$18\% \pm11/2>+10\% \pm9/2>+12\% \mp3/2>+$
						25% ∓5/2>
341	490	0.05	0.26	16.37	40	$13\% \pm9/2>+23\% \pm3/2>+23\% \pm1/2>$
373	536	0.05	0.30	17.18	41	$14\% \pm 5/2>+11\% \pm 3/2>+37\% \mp 1/2>+$
						13% ∓3/2>

Table S14. SA-CASSCF/RASSI calculated electronic states for 1.

![](_page_35_Figure_4.jpeg)

Fig. S53. The principal magnetic axis of the ground Kramer's doublet of 1.

![](_page_35_Figure_6.jpeg)

Fig. S54. Ab initio calculated electronic states of the J = 15/2 manifold of the  ${}^{6}H_{15/2}$  term of Dy<sup>III</sup> in 1.

Energy (cm <sup>-1</sup> )	Energy (K)	gx	<i>g</i> y	gz	<i>g</i> <sub>z</sub> Angle (°)	Wavefunction
0	0	0.00	0.00	19.87		89% ±15/2>+10% ±13/2>
150	215	1.90	4.36	13.69	57	$19\% \pm13/2>+13\% \pm5/2>+39\% \pm3/2>+$
						19% ±1/2>
160	230	4.04	5.30	9.96	89	$36\% \pm13/2>+42\% \pm1/2>$
183	263	0.40	3.02	8.23	83	$23\% \pm13/2>+28\% \pm5/2>+13\% \pm3/2>+$
						$20\%  \pm 1/2>$
209	300	0.38	4.38	7.22	85	$32\% \pm7/2>+11\% \pm5/2>+30\% \pm3/2>$
238	342	0.52	1.81	13.64	29	60% ±11/2>
248	356	1.25	3.55	10.99	51	$14\% \pm11/2>+43\% \pm9/2>+19\% \pm5/2>$
286	411	0.02	0.29	17.69	53	$34\% \pm9/2>+45\% \pm7/2>+17\% \pm5/2>$

Table S15. SA-CASSCF/RASSI calculated electronic states for 2.

![](_page_36_Figure_3.jpeg)

Fig. S55. The principal magnetic axis of the ground Kramer's doublet of 2.

![](_page_36_Figure_5.jpeg)

Fig. S56. Ab initio calculated electronic states of the J = 15/2 manifold of the  ${}^{6}H_{15/2}$  term of Dy<sup>III</sup> in 2.

Energy	Energy	gx	$g_{\rm v}$	gz	$g_z$ Angle (°)	Wavefunction
(cm <sup>-1</sup> )	(K)	-	- •	-		
0	0	0.00	0.00	19.88		92%  ±15/2>
167	240	0.08	0.18	15.79	9.4	72% ±13/2>
186	267	2.19	8.21	10.99	87	$30\%  \pm 3/2 > +48\%  \pm 1/2 >$
210	302	0.11	4.39	6.33	79	$11\% \pm 7/2 > +32\% \pm 5/2 > +10\% \pm 3/2 > +$
						$26\% \pm 1/2>$
237	340	0.69	5.15	8.25	89	$26\% \pm7/2>+27\% \pm3/2>$
256	368	0.43	1.91	12.80	64	$71\% \pm11/2>$
273	392	1.34	3.97	10.21	45	$54\% \pm9/2>+24\% \pm5/2>$
312	448	0.03	0.29	17.87	39	$27\%$ $\pm 9/2 > +47\%$ $\pm 7/2 > +20\%$ $\pm 5/2 >$

Table S16. SA-CASSCF/RASSI calculated electronic states for 3.

![](_page_37_Figure_3.jpeg)

Fig. S57. The principal magnetic axis of the ground Kramer's doublet of 3.

![](_page_37_Figure_5.jpeg)

Fig. S58. Ab initio calculated electronic states of the J = 15/2 manifold of the  ${}^{6}H_{15/2}$  term of Dy<sup>III</sup> in 3.

Energy	$g_{\rm x}$	$g_{\mathrm{y}}$	gz	$g_z$ Angle (°)	Wavefunction	
(K)						
0	0.00	0.00	19.88	-	91% ±15/2>	
253	0.01	0.05	16.78	2.7	81% ±13/2>	
310	1.64	7.25	12.54	74	$27\%$ $\pm 3/2$ >+25% $\pm 1/2$ >+18% $\mp 1/2$ >	
342	0.11	4.40	7.68	89	$21\% \pm 5/2>+26\% \pm 1/2>+10\% \mp 1/2>+$	
					$12\% \mp 5/2 > +10\% \mp 7/2 >$	
376	1.25	5.39	11.07	37	$24\% \pm 11/2>+14\% \pm 3/2>+12\% \mp 3/2>+$	
					$10\% \mp7/2>+11\% \mp11/2>$	
395	0.88	2.77	10.13	52	$47\%  \pm 11/2 > +18\%  \pm 7/2 > +11\%  \pm 1/2 >$	
427	1.62	4.25	10.05	87	$55\%  \pm 9/2 > +23\%  \pm 5/2 > +12\%  \pm 3/2 >$	
486	0.07	0.32	18.01	80	$24\%  \pm 9/2 > +48\%  \pm 7/2 > +21\%  \pm 5/2 >$	
	Energy (K) 0 253 310 342 376 395 427 486	Energy $g_x$ (K)         0         0.00           253         0.01         310         1.64           342         0.11         376         1.25           395         0.88         427         1.62           486         0.07	Energy $g_x$ $g_y$ (K)         0         0.00         0.00           253         0.01         0.05         310         1.64         7.25           342         0.11         4.40         376         1.25         5.39           395         0.88         2.77         427         1.62         4.25           486         0.07         0.32         0.32         0.30	Energy $g_x$ $g_y$ $g_z$ (K)         0         0.00         0.00         19.88           253         0.01         0.05         16.78           310         1.64         7.25         12.54           342         0.11         4.40         7.68           376         1.25         5.39         11.07           395         0.88         2.77         10.13           427         1.62         4.25         10.05           486         0.07         0.32         18.01	Energy $g_x$ $g_y$ $g_z$ $g_z$ Angle (°)           (K)         0         0.00         0.00         19.88         -           253         0.01         0.05         16.78         2.7           310         1.64         7.25         12.54         74           342         0.11         4.40         7.68         89           376         1.25         5.39         11.07         37           395         0.88         2.77         10.13         52           427         1.62         4.25         10.05         87           486         0.07         0.32         18.01         80	

Table S17. SA-CASSCF/RASSI calculated electronic states for 4.

![](_page_38_Figure_3.jpeg)

Fig. S59. The principal magnetic axis of the ground Kramer's doublet of 4.

![](_page_38_Figure_5.jpeg)

Fig. S60. Ab initio calculated electronic states of the J = 15/2 manifold of the  ${}^{6}H_{15/2}$  term of Dy<sup>III</sup> in 4.

Energy (cm <sup>-1</sup> )	Energy (K)	g <sub>x</sub>	$g_{ m y}$	gz	g <sub>z</sub> Angle (°)	Wavefunction
0	0	0.00	0.00	19.87		89% ±15/2>+10% ±13/2>
165	237	0.18	0.29	15.34	15	$68\% \pm13/2>+11\% \pm3/2>$
180	258	2.60	8.34	10.32	89	27% ±3/2>+49% ±1/2>
205	294	0.16	4.27	6.33	34	$10\% \pm7/2>+32\% \pm5/2>+11\% \pm3/2>+$
						$28\% \pm 1/2>$
232	333	0.61	5.01	7.94	68	$10\% \pm 9/2 > \pm 29\% \pm 7/2 > \pm 29\% \pm 3/2 >$
253	363	0.35	1.87	13.12	79	72% ±11/2>
268	385	1.29	3.92	10.29	55	$53\%  \pm 9/2 > +23\%  \pm 5/2 > +10\%  \pm 3/2 >$
307	441	0.01	0.29	17.84	62	$28\% \pm9/2>+47\% \pm7/2>+20\% \pm5/2>$

Table S18. SA-CASSCF/RASSI calculated electronic states for 5.

![](_page_39_Figure_3.jpeg)

Fig. S61. The principal magnetic axis of the ground Kramer's doublet of 5.

![](_page_39_Figure_5.jpeg)

Fig. S62. Ab initio calculated electronic states of the J = 15/2 manifold of the  ${}^{6}H_{15/2}$  term of Dy<sup>III</sup> in 5.

Energy	Energy	gx	$g_{ m y}$	gz	<i>g</i> <sub>z</sub> Angle (°)	Wavefunction
(cm <sup>-1</sup> )	(K)					
0	0	0.00	0.00	19.91		93% ±15/2>
204	293	0.00	0.01	17.29	1.3	88% ±13/2>
307	441	1.58	2.09	14.02	27	70% ±11/2>+11% ±1/2>
334	480	0.12	0.90	16.47	81	$13\% \pm11/2>+16\% \pm7/2>+29\% \pm5/2>+$
						25% ±3/2>
342	491	2.12	6.11	9.71	87	$20\% \pm9/2>+13\% \pm7/2>+11\% \pm3/2>+$
						$26\% \pm1/2>+11\% \mp1/2>$
365	524	0.99	5.86	9.01	57	$18\% \pm9/2>+10\% \pm7/2>+13\% \pm3/2>+$
						$12\% \pm 1/2>+19\% \mp 1/2>+11\% \mp 9/2>$
388	557	1.98	4.99	10.39	34	$31\% \pm9/2>+13\% \pm7/2>+10\% \pm5/2>+$
						24% ±3/2>
431	619	0.22	0.56	18.24	83	$41\% \pm7/2>+37\% \pm5/2>+11\% \pm3/2>$

Table S19. SA-CASSCF/RASSI calculated electronic states for 6.

![](_page_40_Figure_3.jpeg)

Fig. S63. The principal magnetic axis of the ground Kramer's doublet of 6.

![](_page_40_Figure_5.jpeg)

Fig. S64. Ab initio calculated electronic states of the J = 15/2 manifold of the  ${}^{6}H_{15/2}$  term of Dy<sup>III</sup> in 6.

Energy	Energy	$g_{\rm x}$	$g_{\mathrm{y}}$	g <sub>z</sub>	<i>g</i> <sub>z</sub> Angle (°)	Wavefunction
(cm <sup>-1</sup> )	(K)					
0	0	0.00	0.00	19.79		94.0% ±15/2>
222	319	2.56	5.96	9.83		$10\% \pm13/2>+15\% \pm9/2>+27\% \pm7/2>+$
						34%  ±5/2>
236	339	0.72	5.11	8.40		33% ±7/2>+126% ∓3/2>
263	378	0.55	4.40	10.47		$10\% \pm13/2>+15\% \pm11/2>+39\% \pm9/2>$
269	386	0.92	2.49	11.26		$21\% \pm 5/2>+23\% \pm 1/2>+10\% \mp 1/2>+$
						11%  ∓3/2>
294	422	1.15	4.36	7.55		$14\%  \pm 13/2 > +26\%  \mp 1/2 > +18\%  \mp 3/2 >$
306	440	1.02	6.56	10.44		$48\%   \pm 13/2 > +15\%   \pm 7/2 > +11\%   \mp 1/2 >$
334	480	0.64	1.03	16.28		$39\% \pm11/2>+11\% \pm9/2>+23\% \mp11/2>$

Table S20. SA-CASSCF/RASSI calculated electronic states for 7.

![](_page_41_Figure_3.jpeg)

Fig. S65. The principal magnetic axis of the ground Kramer's doublet of 7.

![](_page_41_Figure_5.jpeg)

Fig. S66. Ab initio calculated electronic states of the J = 15/2 manifold of the  ${}^{6}H_{15/2}$  term of Dy<sup>III</sup> in 7.

Energy	Energy	g <sub>x</sub>	$g_{\mathrm{y}}$	gz	<i>g</i> <sub>z</sub> Angle (°)	Wavefunction
(cm <sup>-1</sup> )	(K)					
0	0	0.00	0.00	19.82		95.9% ±15/2>
289	416	0.20	0.99	13.61	11	$49\%   \pm 13/2 > +24\%   \pm 9/2 > +10\%   \pm 7/2 > +$
						$12\%  \pm 5/2>$
318	457	1.55	2.95	9.13	12	$27\% \pm11/2>+32\% \pm7/2>+10\% \pm5/2>+$
						$17\%  \pm 3/2>$
350	503	3.50	5.81	8.26	15	$33\%  \pm 13/2 > +21\%  \pm 5/2 > +15\%  \pm 1/2 >$
388	558	2.77	4.34	10.76	80	$15\% \pm 11/2>+12\% \pm 9/2>+15\% \pm 1/2>+$
						11% ∓11/2>
436	627	0.88	1.48	13.48	71	$21\% \pm11/2>+22\% \mp9/2>$
464	667	1.28	1.49	17.38	64	$17\% \pm 9/2>+14\% \pm 7/2>+16\% \pm 5/2>+$
						$10\% \mp 3/2 > +14\% \mp 7/2 >$
550	791	0.06	0.09	19.59	89	$22\%  \pm 3/2 > +42\%  \mp 1/2 > +10\%  \mp 4/2 > +$
						15% 75/2>

 Table S21. SA-CASSCF/RASSI calculated electronic states for 8.

 $^{\rm a}$  Only components with >10% contribution are given, rounded to the nearest percent.

Table S22. SA-CASSCF/RASSI calculated electronic states for 9.

Energy	Energy	gx	$g_{\mathrm{y}}$	gz	g <sub>z</sub> Angle (°)	Wavefunction
(cm <sup>-1</sup> )	(K)					
0	0	0.00	0.00	19.81		95.3% ±15/2>
269	386	0.77	3.28	12.39	17	$30\% \pm13/2>+23\% \pm9/2>+22\% \pm7/2>+$
						$17\%  \pm 5/2>$
288	414	0.51	3.09	10.06	23	$18\% \pm11/2>+26\% \pm7/2>+11\% \pm5/2>+$
						$12\%  \pm 3/2>$
317	455	3.95	5.96	10.10	20	$38\% \pm13/2>+14\% \pm5/2>+15\% \pm3/2>+$
						$15\% \pm 1/2>$
336	483	2.17	4.03	9.82	87	$10\% \pm13/2>+10\% \pm11/2>+15\% \pm9/2>+$
						$15\% \pm 1/2>+11\% \mp 11/2>$
365	524	0.24	2.16	13.56	76	$10\% \pm7/2>+10\% \pm5/2>+12\% \pm3/2>+$
						$12\%  \pm 1/2 > +12\%  \mp 3/2 > +11\%  \mp 5/2 >$
383	550	0.18	1.09	17.15	37	$41\%  \pm 11/2 > +31\%  \pm 9/2 > +13\%  \pm 7/2 >$
429	616	0.29	0.44	19.05	89	$10\% \pm 5/2>+37\% \pm 1/2>+24\% \mp 3/2>$

![](_page_43_Figure_0.jpeg)

Fig. S67. The principal magnetic axis of the ground Kramer's doublet of 9.

![](_page_43_Figure_2.jpeg)

Fig. S68. Ab initio calculated electronic states of the J = 15/2 manifold of the  ${}^{6}H_{15/2}$  term of Dy<sup>III</sup> in 9.

Table S23. SA-CASSCF/RASSI calculated electronic states for 10.

Energy	Energy	gx	$g_{\mathrm{y}}$	gz	<i>g</i> <sub>z</sub> Angle (°)	Wavefunction
(cm <sup>-1</sup> )	(K)					
0	0	0.00	0.00	19.78		95.08% ±15/2>
244	350	0.14	2.03	13.02	14	$17\% \pm13/2>+24\% \pm9/2>+18\% \pm7/2>+$
						26% ±5/2>
257	369	0.94	2.99	12.14	37	$13\% \pm11/2>+32\% \pm7/2>+12\% \pm5/2>+$
						23% ±3/2>
294	422	4.73	5.95	9.88	29	$29\% \pm13/2>+12\% \pm5/2>+10\% \pm3/2>+$
						$16\%  \pm 1/2 > +10\%  \mp 1/2 >$
321	461	0.41	2.89	10.57	89	$25\% \pm 13/2>+10\% \pm 9/2>+15\% \mp 11/2>$
353	507	0.00	2.67	13.58	62	$13\% \pm13/2>+10\% \pm9/2>+12\% \pm7/2>+$
						$10\%  \pm 3/2 > +10\%  \mp 1/2 > +10\%  \mp 3/2 > +$
						13% ∓5/2>
375	539	0.62	1.30	17.49	33	$41\%  \pm 11/2 > +30\%  \pm 9/2 > +15\%  \pm 7/2 >$
422	606	0.09	0.26	19.34	89	$14\% \pm 5/2>+11\% \pm 3/2>+34\% \pm 1/2>+$
						19% ∓3/2>

![](_page_44_Picture_0.jpeg)

Fig. S69. The principal magnetic axis of the ground Kramer's doublet of 10.

![](_page_44_Figure_2.jpeg)

Fig. S70. Ab initio calculated electronic states of the J = 15/2 manifold of the  ${}^{6}H_{15/2}$  term of Dy<sup>III</sup> in 10.

Crystal Field Parameter	Value / cm <sup>-1</sup>
$B_2^{-2}$	-0.20140937737544E+00
$B_{2}^{-1}$	-0.61916186433164E+00
$B_{2}^{0}$	-0.10609521340021E+01
$B_2^1$	0.16557453195910E+00
$B_2^2$	0.81228443784434E+00
$B_{4}^{-4}$	0.15523232904314E-01
$B_{4}^{-3}$	0.87746144073827E-01
$B_{4}^{-2}$	-0.74578023994291E-02
$B_{4}^{-1}$	0.11335859513893E-01
$B_4^0$	0.82985231115575E-03
$B_4^1$	-0.79311026458078E-03
$B_4^2$	0.37914444739304E-02
$B_4^3$	0.36367146818877E-01
$B_4^4$	-0.33456744272099E-01
$B_{6}^{-6}$	-0.34150914385560E-04
$B_{6}^{-5}$	-0.61852158116271E-03
$B_{6}^{-4}$	-0.17229173037412E-04
$B_{6}^{-3}$	-0.24685414761921E-03
$B_{6}^{-2}$	0.74915855744264E-05
$B_{6}^{-1}$	-0.15840496633539E-03
$B_6^0$	-0.19856465035579E-04
$B_6^1$	0.26660775045830E-04
$B_{6}^{2}$	-0.75707217400793E-04
$B_{6}^{3}$	0.60511422422283E-05
$B_{6}^{4}$	0.21229398181935E-04
$B_{6}^{5}$	-0.28114727718702E-03
$B_{6}^{6}$	-0.40281052968550E-04

 Table S24. Ab initio
 calculated crystal field parameters for 1.

Crystal Field Parameter	Value / cm <sup>-1</sup>
$B_2^{-2}$	-0.10860332915291E-01
$B_2^{-1}$	-0.99897685672628E-02
$B_{2}^{0}$	-0.08032547373796E+01
$B_2^1$	0.14059707576645E-01
$B_{2}^{2}$	0.02563937821253E+00
$B_{4}^{-4}$	-0.75767680942513E-03
$B_4^{-3}$	0.33998996798161E-03
$B_{4}^{-2}$	0.71820624211116E-03
$B_{4}^{-1}$	-0.20196641613823E-02
$B_4^0$	-0.52166117974776E-02
$B_4^1$	0.23942957512731E-01
$B_4^2$	-0.29284840309877E-02
$B_{4}^{3}$	-0.68631514856063E-02
$B_4^4$	-0.16757145033051E-04
$B_{6}^{-6}$	-0.19326559548162E-04
$B_{6}^{-5}$	-0.10049018826113E-03
$B_{6}^{-4}$	-0.14989893161006E-04
$B_{6}^{-3}$	-0.11084759181051E-04
$B_{6}^{-2}$	0.59348731392622E-06
$B_{6}^{-1}$	0.24231886021961E-04
$B_6^0$	0.49354474895370E-05
$B_6^1$	0.54944436541463E-05
$B_6^2$	-0.20968469259837E-04
$B_{6}^{3}$	-0.52516476740811E-04
$B_{6}^{4}$	-0.19593313305189E-04
$B_{6}^{5}$	-0.41803030599367E-03
$B_6^6$	0.22012053393123E-04

 Table S25. Ab initio
 calculated crystal field parameters for 2.

Crystal Field Parameter	Value / cm <sup>-1</sup>
$B_2^{-2}$	-0.11369458741384E-01
$B_2^{-1}$	-0.87174978174339E-02
$B_2^0$	-0.10133158746343E+01
$B_{2}^{1}$	0.13157437436196E-01
$B_{2}^{2}$	0.03183515446464E+00
$B_{4}^{-4}$	0.74818173660896E-03
$B_{4}^{-3}$	-0.86497421923558E-03
$B_4^{-2}$	0.98662644529249E-03
$B_{4}^{-1}$	0.94532047486863E-02
$B_4^0$	-0.82013919621240E-02
$B_4^1$	0.73978608837350E-01
$B_4^2$	0.53212674944661E-02
$B_4^3$	-0.47630530588794E-02
$B_4^4$	0.25826202861499E-04
$B_{6}^{-6}$	-0.22580370684154E-04
$B_{6}^{-5}$	-0.94250138790811E-03
$B_{6}^{-4}$	0.78129738294519E-04
$B_{6}^{-3}$	0.14825558990706E-04
$B_{6}^{-2}$	-0.61218214759137E-06
$B_{6}^{-1}$	-0.11976969386451E-04
$B_{6}^{0}$	0.80579312553163E-05
$B_6^1$	-0.55148044296074E-05
$B_{6}^{2}$	0.72154521676711E-04
$B_{6}^{3}$	-0.46227108370512E-04
$B_{6}^{4}$	0.68347040044609E-04
$B_{6}^{5}$	-0.30196860083379E-03
$B_{6}^{6}$	0.50897968043573E-04

 Table S26. Ab initio calculated crystal field parameters for 3.

Crystal Field Parameter	Value / cm <sup>-1</sup>
$B_2^{-2}$	-0.10698745319994E-01
$B_2^{-1}$	-0.85112974543661E-02
$B_{2}^{0}$	-0.12112084733694E+01
$B_{2}^{1}$	0.36128661418333E-02
$B_{2}^{2}$	0.67999153302516E-02
$B_{4}^{-4}$	-0.38490800859872E-03
$B_4^{-3}$	0.89496555516961E-03
$B_{4}^{-2}$	0.61550725151318E-03
$B_{4}^{-1}$	0.37523002075031E-02
$B_4^0$	-0.52324518279638E-02
$B_4^1$	-0.24868354778737E-01
$B_4^2$	0.89714629545341E-02
$B_4^3$	0.10644589245785E-02
$B_4^4$	-0.90547674652188E-04
$B_{6}^{-6}$	-0.61244255676865E-04
$B_{6}^{-5}$	0.28882169802673E-03
$B_{6}^{-4}$	0.21146837463602E-04
$B_{6}^{-3}$	-0.79887017202563E-04
$B_{6}^{-2}$	0.88563783406279E-06
$B_{6}^{-1}$	0.15620307328645E-04
$B_{6}^{0}$	0.33859019149095E-05
$B_6^1$	-0.51598162143491E-05
$B_6^2$	-0.12306321309879E-04
$B_{6}^{3}$	-0.47474471537862E-04
$B_6^4$	0.85201917651574E-04
$B_{6}^{5}$	0.96338287123944E-03
$B_6^6$	-0.59569772412069E-04

 Table S27. Ab initio
 calculated crystal field parameters for 4.

Crystal Field Parameter	Value / cm <sup>-1</sup>
B_2^{-2}	0.43123904732056E-01
$B_2^{-1}$	0.64292725215200E-02
$B_{2}^{0}$	-0.97325473737961E+00
$B_2^1$	0.22048912236933E-02
$B_2^2$	0.48191147015895E-02
$B_{4}^{-4}$	-0.66018648722674E-03
$B_{4}^{-3}$	-0.34010105447378E-03
$B_{4}^{-2}$	0.35835115937516E-03
$B_{4}^{-1}$	0.66797851207665E-02
$B_4^0$	-0.11076042703353E-02
$B_4^1$	0.74415713269263E-01
$B_4^2$	-0.89273732679430E-02
$B_4^3$	0.11773899551481E-02
$B_4^4$	0.36009414554573E-04
$B_{6}^{-6}$	-0.25177716470789E-04
$B_{6}^{-5}$	-0.37177104232832E-03
$B_{6}^{-4}$	0.22612946406007E-04
$B_{6}^{-3}$	0.30073322984390E-04
$B_{6}^{-2}$	-0.11380763503257E-06
$B_{6}^{-1}$	0.77983165588229E-04
$B_{6}^{0}$	0.62956051444634E-05
$B_6^1$	0.64114560005254E-05
$B_{6}^{2}$	-0.66323934148531E-04
$B_{6}^{3}$	-0.52964645335450E-04
$B_{6}^{4}$	-0.57662061119917E-04
$B_{6}^{5}$	0.29691632152535E-03
$B_{6}^{6}$	0.67717296406626E-04

 Table S28. Ab initio calculated crystal field parameters for 5.

Crystal Field Parameter	Value / cm <sup>-1</sup>
	0.83550540653522E-01
$B_2^{-1}$	0.38963494747877E-02
$B_{2}^{0}$	-0.19132547373796E+01
$B_2^1$	0.69292452903464E-02
$B_{2}^{2}$	-0.32308932170272E-02
$B_{4}^{-4}$	-0.42937284822110E-03
$B_{4}^{-3}$	-0.51140891187824E-03
$B_{4}^{-2}$	0.43662222949788E-03
$B_{4}^{-1}$	0.89254466267302E-02
$B_4^0$	-0.66879837347660E-02
$B_4^1$	0.39707790210377E-01
$B_4^2$	0.93518337707500E-02
$B_4^3$	0.82973712200764E-02
$B_4^4$	0.90335459930356E-04
$B_{6}^{-6}$	-0.79019231118727E-04
$B_{6}^{-5}$	-0.22863104410935E-03
$B_{6}^{-4}$	0.29402656024322E-04
$B_{6}^{-3}$	0.94305928214452E-04
$B_{6}^{-2}$	0.31141180822160E-06
$B_{6}^{-1}$	0.59765556047204E-04
$B_{6}^{0}$	0.87675837483256E-05
$B_6^1$	-0.33037880263291E-05
$B_{6}^{2}$	0.65223663470242E-04
$B_{6}^{3}$	0.45628794333897E-04
$B_{6}^{4}$	-0.90050886354874E-04
$B_{6}^{5}$	-0.68943507275543E-03
$B_{6}^{6}$	-0.92566073921043E-04

 Table S29. Ab initio
 calculated crystal field parameters for 6.

Crystal Field Parameter	Value / cm <sup>-1</sup>
$B_2^{-2}$	0.91816361632663E-01
$B_2^{-1}$	0.52904619676992E+00
$B_{2}^{0}$	-0.90825960233342E+00
$B_2^1$	0.64711256481241E+00
$B_{2}^{2}$	-0.11071205153130E+00
$B_{4}^{-4}$	-0.82095586159266E-02
$B_{4}^{-3}$	-0.60090272463858E-02
$B_4^{-2}$	0.43665379260201E-03
$B_{4}^{-1}$	0.17403876788448E-02
$B_4^0$	-0.54933839165605E-01
$B_4^1$	0.31014772690832E-03
$B_4^2$	0.73781905414070E-02
$B_4^3$	0.48679023799486E-02
$B_4^4$	0.38650872369762E-02
$B_{6}^{-6}$	-0.88108505436684E-04
$B_{6}^{-5}$	-0.13055284549482E-03
$B_{6}^{-4}$	0.87858934479299E-05
$B_{6}^{-3}$	0.33847712255083E-04
$B_{6}^{-2}$	0.69753214376978E-04
$B_{6}^{-1}$	-0.96518202056176E-04
$B_6^0$	0.99705524400341E-04
$B_6^1$	-0.10723511779215E-03
$B_{6}^{2}$	-0.28545141124632E-03
$B_{6}^{3}$	0.20032011275180E-03
$B_{6}^{4}$	0.93712748198303E-03
$B_{6}^{5}$	-0.49439743622206E-02
$B_6^6$	-0.72812648618127E-03

 Table S30. Ab initio calculated crystal field parameters for 7.

Crystal Field Parameter	Value / cm <sup>-1</sup>
	0.67574222100026E-01
$B_2^{-1}$	0.14084193910491E+00
$B_{2}^{0}$	-0.19711658539994E+01
$B_2^1$	0.28668035397265E+00
$B_2^2$	-0.20672867544930E+00
$B_{4}^{-4}$	0.35964733179041E-02
$B_{4}^{-3}$	-0.42031104953003E-02
$B_{4}^{-2}$	-0.76485659809604E-03
$B_{4}^{-1}$	-0.35760701978053E-02
$B_4^0$	-0.17508113435075E-01
$B_4^1$	-0.84703416376927E-03
$B_4^2$	0.13458278902698E-02
$B_4^3$	0.33423579793977E-02
$B_4^4$	-0.24066544186009E-02
$B_{6}^{-6}$	0.97016951959562E-04
$B_{6}^{-5}$	-0.43248697502466E-03
$B_{6}^{-4}$	0.51350185974349E-05
$B_{6}^{-3}$	-0.27547414475068E-04
$B_{6}^{-2}$	0.30824358422438E-04
$B_{6}^{-1}$	-0.29889169434938E-04
$B_{6}^{0}$	0.13715302895895E-04
$B_6^1$	0.13959846200552E-03
$B_{6}^{2}$	-0.14823738771059E-03
$B_{6}^{3}$	-0.16748494689012E-03
$B_{6}^{4}$	0.10945315196673E-03
$B_{6}^{5}$	0.10862440370663E-02
$B_{6}^{6}$	-0.32590987903891E-03

 Table S31. Ab initio
 calculated crystal field parameters for 8.

Crystal Field Parameter	Value / cm <sup>-1</sup>
$B_2^{-2}$	0.67409740197472E-01
$B_2^{-1}$	0.22738838547375E+00
$B_{2}^{0}$	-0.12767977138378E+01
$B_2^1$	0.54356795276980E+00
$B_{2}^{2}$	-0.17673397874136E+00
$B_{4}^{-4}$	0.31248745094053E-02
$B_4^{-3}$	-0.46262678150087E-02
$B_{4}^{-2}$	0.93047320409677E-03
$B_{4}^{-1}$	0.54012417199555E-02
$B_4^0$	-0.30834275174420E-01
$B_4^1$	0.27708761969115E-03
$B_4^2$	0.23622245900333E-02
$B_4^3$	-0.62835830918047E-03
$B_4^4$	-0.19209607099183E-02
$B_{6}^{-6}$	0.70733292063232E-04
$B_{6}^{-5}$	-0.99814373974222E-03
$B_{6}^{-4}$	-0.23481970350258E-05
$B_{6}^{-3}$	0.74742546011693E-04
$B_{6}^{-2}$	0.63024612562730E-05
$B_{6}^{-1}$	0.44997550921980E-04
$B_{6}^{0}$	0.91070069035049E-04
$B_6^1$	-0.35548536467831E-03
$B_{6}^{2}$	-0.51184212844818E-03
$B_{6}^{3}$	0.98273063015657E-03
$B_{6}^{4}$	0.45775563009083E-03
$B_{6}^{5}$	-0.42364663749467E-02
$B_6^6$	-0.53442855374887E-04

 Table S32. Ab initio
 calculated crystal field parameters for 9.

Crystal Field Parameter	Value / cm <sup>-1</sup>
B_2^{-2}	0.39690229285042E-01
$B_2^{-1}$	0.82542205161880E+00
$B_{2}^{0}$	-0.13722929773922E+01
$B_2^1$	0.31506565457675E+00
$B_{2}^{2}$	-0.13648198627866E+00
$B_{4}^{-4}$	-0.35058235595934E-02
$B_{4}^{-3}$	0.23459281439427E-02
$B_{4}^{-2}$	0.56534160336013E-03
$B_{4}^{-1}$	-0.85213507832958E-02
$B_4^0$	-0.91750391214154E-01
$B_4^1$	0.12749822034966E-03
$B_4^2$	0.18645733422600E-02
$B_4^3$	0.89145776347722E-03
$B_4^4$	-0.84709495969582E-02
$B_{6}^{-6}$	-0.10684864206705E-04
$B_{6}^{-5}$	-0.76893372812773E-04
$B_{6}^{-4}$	0.56204247181303E-05
$B_{6}^{-3}$	0.81018849266692E-04
$B_{6}^{-2}$	-0.46500307535752E-05
$B_{6}^{-1}$	0.20815828186460E-04
$B_{6}^{0}$	0.72812648618127E-04
$B_6^1$	0.63872314055915E-03
$B_{6}^{2}$	0.13697665331420E-03
$B_{6}^{3}$	-0.89084464360493E-03
$B_{6}^{4}$	0.15288004996255E-02
$B_{6}^{5}$	0.56218227001372E-03
$B_{6}^{6}$	-0.28229475675616E-04

 Table S33. Ab initio
 calculated crystal field parameters for 10.

	$ +\frac{15}{2}>$	$ -\frac{15}{2}>$	+a>	-a>	+b>	-b>	+c>	-c>	+d>	-d>	+e>	-e>	+f>	-f>	+g>	-g>
$ +\frac{15}{2}>$		6.4E-01	2.4E-01	1.0E-02	5.4E-02	1.7E-01	1.0E-02	2.2E-01	2.1E-01	3.4E-01	1.5E+00	1.6E-01	2.2E-02	6.3E-01	3.4E-02	2.6E-01
$ -\frac{15}{2}>$	6.4E-01		1.0E-02	2.4E+00	1.7E-01	5.4E-02	2.2E-01	1.0E-02	3.4E-01	2.1E-01	1.6E-01	1.5E+00	6.3E-01	2.2E-02	2.6E-01	3.4E-02
+a>	2.4E-01	1.0E-02		5.2E-02	2.2E-01	2.9E+00	6.0E-02	1.4E+00	3.3E-01	7.7E-01	5.5E-01	4.6E-02	3.7E-03	1.1E-01	8.7E-03	7.8E-02
-a>	1.0E-02	2.4E+00	5.2E-02		2.9E+00	2.2E-01	1.4E+00	6.0E-02	7.7E-01	3.3E-01	4.6E-02	5.5E-01	1.1E-01	3.7E-03	7.8E-02	8.7E-03
+b>	5.4E-02	1.7E-01	2.2E-01	2.9E+00		1.9E+00	7.5E+00	1.2E+00	5.0E-01	8.2E-01	9.4E-02	3.8E-01	4.7E-02	2.2E-02	3.4E-02	8.1E-02
-b>	1.7E-01	5.4E-02	2.9E+00	2.2E-01	1.9E+00		1.2E+00	7.5E+00	8.2E-01	5.0E-01	3.8E-01	9.4E-02	2.2E-02	4.7E-02	8.1E-02	3.4E-02
+c>	1.0E-02	2.2E-01	6.0E-02	1.4E+00	7.5E+00	1.2E+00		4.0E+00	1.0E+01	2.9E+00	7.0E-01	1.2E+00	9.3E-02	1.2E-01	1.7E-02	9.3E-02
-C>	2.2E-01	1.0E-02	1.4E+00	6.0E-02	1.2E+00	7.5E+00	4.0E+00		2.9E+00	1.0E+01	1.2E+00	7.0E-01	1.2E-01	9.3E-02	9.3E-02	1.7E-02
+d>	2.1E-01	3.4E-01	3.3E-01	7.7E-01	5.0E-01	8.2E-01	1.0E+01	2.9E+00		6.6E+00	4.0E+00	6.5E+00	6.0E-01	5.8E-01	9.6E-01	6.3E-01
-d>	3.4E-01	2.1E-01	7.7E-01	3.3E-01	8.2E-01	5.0E-01	2.9E+00	1.0E+01	6.6E+00		6.5E+00	4.0E+00	5.8E-01	6.0E-01	6.3E-01	9.6E-01
+e>	1.5E+00	1.6E-01	5.5E-01	4.6E-02	9.4E-02	3.8E-01	7.0E-01	1.2E+00	4.0E+00	6.5E+00		5.8E+00	6.3E-01	4.2E+00	8.3E-01	1.8E+00
-e>	1.6E-01	1.5E+00	4.6E-02	5.5E-01	3.8E-01	9.4E-02	1.2E+00	7.0E-01	6.5E+00	4.0E+00	5.8E+00		4.2E+00	6.3E-01	1.8E+00	8.3E-01
+f>	2.2E-02	6.3E-01	3.7E-03	1.1E-01	4.7E-02	2.2E-02	9.3E-02	1.2E-01	6.0E-01	5.8E-01	6.3E-01	4.2E+00		2.4E+00	4.9E+00	1.5E+00
-f>	6.3E-01	2.2E-02	1.1E-01	3.7E-03	2.2E-02	4.7E-02	1.2E-01	9.3E-02	5.8E-01	6.0E-01	4.2E+00	6.3E-01	2.4E+00		1.5E+00	4.9E+00
+g>	3.4E-02	2.6E-01	8.7E-03	7.8E-02	3.4E-02	8.1E-02	1.7E-02	9.3E-02	9.6E-01	6.3E-01	8.3E-01	1.8E+00	4.9E+00	1.5E+00		1.1E+01
-g>	2.6E-01	3.4E-02	7.8E-02	8.7E-03	8.1E-02	3.4E-02	9.3E-02	1.7E-02	6.3E-01	9.6E-01	1.8E+00	8.3E-01	1.5E+00	4.9E+00	1.1E+01	

**Table S34**. Average transition magnetic moment elements between the states of 1, given in  $\mu_B^2$ .

	$ +\frac{15}{2}>$	$ -\frac{15}{2}>$	+a>	-a>	+b>	-b>	+c>	-c>	+d>	-d>	+e>	-e>	+f>	-f>	+g>	-g>
$ +\frac{15}{2}>$		3.9E-07	9.1E-01	7.8E-04	6.4E-02	2.4E+00	9.1E-04	1.0E+00	2.4E-02	2.2E-03	6.9E-02	9.4E-03	1.8E-03	2.5E-02	2.7E-02	4.2E-05
$ -\frac{15}{2}>$	3.9E-07		7.8E-04	9.1E-01	2.4E+00	6.4E-02	1.0E+00	9.1E-04	2.2E-03	2.4E-02	9.4E-03	6.9E-02	2.5E-02	1.8E-03	4.2E-05	2.7E-02
+a>	9.1E-01	7.8E-04		3.8E+00	2.7E+00	6.5E+00	9.2E-01	7.4E+00	5.3E-01	1.2E-01	4.2E-01	1.3E-01	3.2E-03	4.3E-01	7.3E-02	7.3E-02
-a>	7.8E-04	9.1E-01	3.8E+00		6.5E+00	2.7E+00	7.4E+00	9.2E-01	1.2E-01	5.3E-01	1.3E-01	4.2E-01	4.3E-01	3.2E-03	7.3E-02	7.3E-02
+b>	6.4E-02	2.4E+00	2.7E+00	6.5E+00		4.8E+00	4.0E+00	1.7E+00	4.0E-01	4.2E+00	7.8E-02	1.9E+00	1.2E+00	1.5E-01	4.8E-02	4.2E-01
-b>	2.4E+00	6.4E-02	6.5E+00	2.7E+00	4.8E+00		1.7E+00	4.0E+00	4.2E+00	4.0E-01	1.9E+00	7.8E-02	1.5E-01	1.2E+00	4.2E-01	4.8E-02
+c>	9.1E-04	1.0E+00	9.2E-01	7.4E+00	4.0E+00	1.7E+00		8.0E-01	4.7E-01	1.1E+01	3.3E-01	2.2E+00	1.7E+00	1.6E-01	2.4E-02	2.9E-01
-C>	1.0E+00	9.1E-04	7.4E+00	9.2E-01	1.7E+00	4.0E+00	8.0E-01		1.1E+01	4.7E-01	2.2E+00	3.3E-01	1.6E-01	1.7E+00	2.9E-01	2.4E-02
+d>	2.4E-02	2.2E-03	5.3E-01	1.2E-01	4.0E-01	4.2E+00	4.7E-01	1.1E+01		2.9E+00	4.7E+00	2.0E+00	4.8E-01	7.0E+00	6.6E-01	1.5E-02
-d>	2.2E-03	2.4E-02	1.2E-01	5.3E-01	4.2E+00	4.0E-01	1.1E+01	4.7E-01	2.9E+00		2.0E+00	4.7E+00	7.0E+00	4.8E-01	1.5E-02	6.6E-01
+e>	6.9E-02	9.4E-03	4.2E-01	1.3E-01	7.8E-02	1.9E+00	3.3E-01	2.2E+00	4.7E+00	2.0E+00		7.4E+00	2.0E+00	5.7E+00	1.8E+00	6.7E-01
-e>	9.4E-03	6.9E-02	1.3E-01	4.2E-01	1.9E+00	7.8E-02	2.2E+00	3.3E-01	2.0E+00	4.7E+00	7.4E+00		5.7E+00	2.0E+00	6.7E-01	1.8E+00
+f>	1.8E-03	2.5E-02	3.2E-03	4.3E-01	1.2E+00	1.5E-01	1.7E+00	1.6E-01	4.8E-01	7.0E+00	2.0E+00	5.7E+00		1.4E+00	1.8E-01	7.4E+00
-f>	2.5E-02	1.8E-03	4.3E-01	3.2E-03	1.5E-01	1.2E+00	1.6E-01	1.7E+00	7.0E+00	4.8E-01	5.7E+00	2.0E+00	1.4E+00		7.4E+00	1.8E-01
+g>	2.7E-02	4.2E-05	7.3E-02	7.3E-02	4.8E-02	4.2E-01	2.4E-02	2.9E-01	6.6E-01	1.5E-02	1.8E+00	6.7E-01	1.8E-01	7.4E+00		6.1E-02
-g>	4.2E-05	2.7E-02	7.3E-02	7.3E-02	4.2E-01	4.8E-02	2.9E-01	2.4E-02	1.5E-02	6.6E-01	6.7E-01	1.8E+00	7.4E+00	1.8E-01	6.1E-02	

Table S35. Average transition magnetic moment elements between the states of 2, given in  $\mu_B^2$ .

	$ +\frac{15}{2}>$	$ -\frac{15}{2}>$	+a>	-a>	+b>	-b>	+c>	-c>	+d>	-d>	+e>	-e>	+f>	-f>	+g>	-g>
$ +\frac{15}{2}>$		1.8E-07	3.8E+00	3.2E-05	1.3E-03	3.4E-01	5.2E-03	2.1E-01	3.4E-03	2.1E-02	8.5E-02	8.1E-04	1.4E-02	1.1E-03	2.0E-02	4.6E-05
$ -\frac{15}{2}>$	1.8E-07		3.2E-05	3.8E+00	3.4E-01	1.3E-03	2.1E-01	5.2E-03	2.1E-02	3.4E-03	8.1E-04	8.5E-02	1.1E-03	1.4E-02	4.6E-05	2.0E-02
+a>	3.8E+00	3.2E-05		3.4E-03	1.1E-01	4.9E+00	1.1E-01	1.9E+00	2.1E-01	1.1E+00	3.3E+00	4.1E-02	1.1E+00	2.6E-02	3.6E-01	9.3E-03
-a>	3.2E-05	3.8E+00	3.4E-03		4.9E+00	1.1E-01	1.9E+00	1.1E-01	1.1E+00	2.1E-01	4.1E-02	3.3E+00	2.6E-02	1.1E+00	9.3E-03	3.6E-01
+b>	1.3E-03	3.4E-01	1.1E-01	4.9E+00		9.6E+00	9.3E+00	4.0E+00	6.4E-01	3.6E-01	1.7E-01	1.4E+00	4.6E-02	2.1E-01	1.1E-01	1.2E-01
-b>	3.4E-01	1.3E-03	4.9E+00	1.1E-01	9.6E+00		4.0E+00	9.3E+00	3.6E-01	6.4E-01	1.4E+00	1.7E-01	2.1E-01	4.6E-02	1.2E-01	1.1E-01
+c>	5.2E-03	2.1E-01	1.1E-01	1.9E+00	9.3E+00	4.0E+00		2.5E+00	1.2E+01	1.2E+00	1.4E-01	2.6E+00	3.6E-01	4.5E-01	3.3E-02	8.1E-02
-C>	2.1E-01	5.2E-03	1.9E+00	1.1E-01	4.0E+00	9.3E+00	2.5E+00		1.2E+00	1.2E+01	2.6E+00	1.4E-01	4.5E-01	3.6E-01	8.1E-02	3.3E-02
+d>	3.4E-03	2.1E-02	2.1E-01	1.1E+00	6.4E-01	3.6E-01	1.2E+01	1.2E+00		5.0E+00	1.5E+00	3.0E+00	9.2E-01	7.7E+00	7.5E-02	6.6E-01
-d>	2.1E-02	3.4E-03	1.1E+00	2.1E-01	3.6E-01	6.4E-01	1.2E+00	1.2E+01	5.0E+00		3.0E+00	1.5E+00	7.7E+00	9.2E-01	6.6E-01	7.5E-02
+e>	8.5E-02	8.1E-04	3.3E+00	4.1E-02	1.7E-01	1.4E+00	1.4E-01	2.6E+00	1.5E+00	3.0E+00		1.1E+00	8.4E+00	1.0E+00	1.9E+00	3.0E-01
-e>	8.1E-04	8.5E-02	4.1E-02	3.3E+00	1.4E+00	1.7E-01	2.6E+00	1.4E-01	3.0E+00	1.5E+00	1.1E+00		1.0E+00	8.4E+00	3.0E-01	1.9E+00
+f>	1.4E-02	1.1E-03	1.1E+00	2.6E-02	4.6E-02	2.1E-01	3.6E-01	4.5E-01	9.2E-01	7.7E+00	8.4E+00	1.0E+00		1.7E+00	7.3E+00	2.1E-01
-f>	1.1E-03	1.4E-02	2.6E-02	1.1E+00	2.1E-01	4.6E-02	4.5E-01	3.6E-01	7.7E+00	9.2E-01	1.0E+00	8.4E+00	1.7E+00		2.1E-01	7.3E+00
+g>	2.0E-02	4.6E-05	3.6E-01	9.3E-03	1.1E-01	1.2E-01	3.3E-02	8.1E-02	7.5E-02	6.6E-01	1.9E+00	3.0E-01	7.3E+00	2.1E-01		2.6E-01
-g>	4.6E-05	2.0E-02	9.3E-03	3.6E-01	1.2E-01	1.1E-01	8.1E-02	3.3E-02	6.6E-01	7.5E-02	3.0E-01	1.9E+00	2.1E-01	7.3E+00	2.6E-01	

Table S36. Average transition magnetic moment elements between the states of 3, given in  $\mu_B^2$ .

	$ +\frac{15}{2}>$	$ -\frac{15}{2}>$	+a>	-a>	+b>	-b>	+c>	-c>	+d>	-d>	+e>	-e>	+f>	-f>	+g>	-g>
$ +\frac{15}{2}>$		9.7E-08	2.2E-05	4.2E+00	2.2E-02	1.0E-01	3.2E-02	3.4E-02	2.1E-02	1.6E-02	1.0E-03	6.7E-02	4.6E-04	9.9E-03	4.2E-05	1.6E-02
$ -\frac{15}{2}>$	9.7E-08		4.2E+00	2.2E-05	1.0E-01	2.2E-02	3.4E-02	3.2E-02	1.6E-02	2.1E-02	6.7E-02	1.0E-03	9.9E-03	4.6E-04	1.6E-02	4.2E-05
+a>	2.2E-05	4.2E+00		6.3E-04	2.4E+00	5.6E-01	4.2E-01	3.9E-01	6.8E-01	1.4E+00	3.0E+00	6.7E-02	8.0E-01	1.1E-02	2.9E-01	2.9E-03
-a>	4.2E+00	2.2E-05	6.3E-04		5.6E-01	2.4E+00	3.9E-01	4.2E-01	1.4E+00	6.8E-01	6.7E-02	3.0E+00	1.1E-02	8.0E-01	2.9E-03	2.9E-01
+b>	2.2E-02	1.0E-01	2.4E+00	5.6E-01		7.6E+00	8.5E+00	5.0E+00	4.9E-01	8.0E-01	1.1E+00	5.9E-01	1.5E-01	4.6E-02	1.3E-01	8.4E-02
-b>	1.0E-01	2.2E-02	5.6E-01	2.4E+00	7.6E+00		5.0E+00	8.5E+00	8.0E-01	4.9E-01	5.9E-01	1.1E+00	4.6E-02	1.5E-01	8.4E-02	1.3E-01
+c>	3.2E-02	3.4E-02	4.2E-01	3.9E-01	8.5E+00	5.0E+00		6.5E+00	3.6E+00	7.0E+00	2.2E+00	3.1E+00	6.8E-01	1.3E-01	6.1E-02	2.6E-02
-c>	3.4E-02	3.2E-02	3.9E-01	4.2E-01	5.0E+00	8.5E+00	6.5E+00		7.0E+00	3.6E+00	3.1E+00	2.2E+00	1.3E-01	6.8E-01	2.6E-02	6.1E-02
+d>	2.1E-02	1.6E-02	6.8E-01	1.4E+00	4.9E-01	8.0E-01	3.6E+00	7.0E+00		1.2E+01	5.5E-01	3.5E+00	4.0E+00	2.2E+00	3.2E-01	4.5E-01
-d>	1.6E-02	2.1E-02	1.4E+00	6.8E-01	8.0E-01	4.9E-01	7.0E+00	3.6E+00	1.2E+01		3.5E+00	5.5E-01	2.2E+00	4.0E+00	4.5E-01	3.2E-01
+e>	1.0E-03	6.7E-02	3.0E+00	6.7E-02	1.1E+00	5.9E-01	2.2E+00	3.1E+00	5.5E-01	3.5E+00		7.9E-01	1.1E+01	1.1E+00	1.7E+00	3.0E-01
-e>	6.7E-02	1.0E-03	6.7E-02	3.0E+00	5.9E-01	1.1E+00	3.1E+00	2.2E+00	3.5E+00	5.5E-01	7.9E-01		1.1E+00	1.1E+01	3.0E-01	1.7E+00
+f>	4.6E-04	9.9E-03	8.0E-01	1.1E-02	1.5E-01	4.6E-02	6.8E-01	1.3E-01	4.0E+00	2.2E+00	1.1E+01	1.1E+00		2.7E+00	7.0E+00	4.3E-01
-f>	9.9E-03	4.6E-04	1.1E-02	8.0E-01	4.6E-02	1.5E-01	1.3E-01	6.8E-01	2.2E+00	4.0E+00	1.1E+00	1.1E+01	2.7E+00		4.3E-01	7.0E+00
+g>	4.2E-05	1.6E-02	2.9E-01	2.9E-03	1.3E-01	8.4E-02	6.1E-02	2.6E-02	3.2E-01	4.5E-01	1.7E+00	3.0E-01	7.0E+00	4.3E-01		3.0E-01
-g>	1.6E-02	4.2E-05	2.9E-03	2.9E-01	8.4E-02	1.3E-01	2.6E-02	6.1E-02	4.5E-01	3.2E-01	3.0E-01	1.7E+00	4.3E-01	7.0E+00	3.0E-01	

Table S37. Average transition magnetic moment elements between the states of 4, given in  $\mu_B^2$ .

	$ +\frac{15}{2}>$	$ -\frac{15}{2}>$	$ +\frac{13}{2}>$	$ -\frac{13}{2}>$	+a>	-a>	+b>	-b>	+c>	-c>	+d>	-d>	+e>	-e>	+f>	-f>
$ +\frac{15}{2}>$		2.1E-07	9.0E-05	3.6E+00	1.5E-03	4.8E-01	1.4E-03	2.8E-01	2.2E-02	2.3E-03	8.4E-02	1.6E-03	1.6E-02	1.0E-03	2.2E-02	1.1E-05
$ -\frac{15}{2}>$	2.1E-07		3.6E+00	9.0E-05	4.8E-01	1.5E-03	2.8E-01	1.4E-03	2.3E-03	2.2E-02	1.6E-03	8.4E-02	1.0E-03	1.6E-02	1.1E-05	2.2E-02
$ +\frac{13}{2}>$	9.0E-05	3.6E+00		1.2E-02	5.7E+00	3.4E-01	2.4E+00	1.3E-01	1.4E-01	1.2E+00	6.9E-02	3.0E+00	2.1E-02	1.1E+00	1.2E-02	3.6E-01
$ -\frac{13}{2}>$	3.6E+00	9.0E-05	1.2E-02		3.4E-01	5.7E+00	1.3E-01	2.4E+00	1.2E+00	1.4E-01	3.0E+00	6.9E-02	1.1E+00	2.1E-02	3.6E-01	1.2E-02
+a>	1.5E-03	4.8E-01	5.7E+00	3.4E-01		1.1E+01	9.6E+00	3.1E+00	3.4E-01	7.8E-01	1.3E-01	1.5E+00	4.3E-02	2.8E-01	9.5E-02	1.5E-01
-a>	4.8E-01	1.5E-03	3.4E-01	5.7E+00	1.1E+01		3.1E+00	9.6E+00	7.8E-01	3.4E-01	1.5E+00	1.3E-01	2.8E-01	4.3E-02	1.5E-01	9.5E-02
+b>	1.4E-03	2.8E-01	2.4E+00	1.3E-01	9.6E+00	3.1E+00		1.3E+01	8.0E-01	1.3E+00	2.1E-01	2.4E+00	3.2E-01	5.6E-01	3.0E-02	1.0E-01
-b>	2.8E-01	1.4E-03	1.3E-01	2.4E+00	3.1E+00	9.6E+00	1.3E+01		1.3E+00	8.0E-01	2.4E+00	2.1E-01	5.6E-01	3.2E-01	1.0E-01	3.0E-02
+c>	2.2E-02	2.3E-03	1.4E-01	1.2E+00	3.4E-01	7.8E-01	8.0E-01	1.3E+00		4.0E+00	3.4E+00	1.3E+00	8.1E+00	7.0E-01	6.8E-01	4.4E-02
-c>	2.3E-03	2.2E-02	1.2E+00	1.4E-01	7.8E-01	3.4E-01	1.3E+00	8.0E-01	4.0E+00		1.3E+00	3.4E+00	7.0E-01	8.1E+00	4.4E-02	6.8E-01
+d>	8.4E-02	1.6E-03	6.9E-02	3.0E+00	1.3E-01	1.5E+00	2.1E-01	2.4E+00	3.4E+00	1.3E+00		1.8E+00	8.0E+00	9.4E-01	1.9E+00	3.2E-01
-d>	1.6E-03	8.4E-02	3.0E+00	6.9E-02	1.5E+00	1.3E-01	2.4E+00	2.1E-01	1.3E+00	3.4E+00	1.8E+00		9.4E-01	8.0E+00	3.2E-01	1.9E+00
+e>	1.6E-02	1.0E-03	2.1E-02	1.1E+00	4.3E-02	2.8E-01	3.2E-01	5.6E-01	8.1E+00	7.0E-01	8.0E+00	9.4E-01		1.8E+00	7.3E+00	2.2E-01
-e>	1.0E-03	1.6E-02	1.1E+00	2.1E-02	2.8E-01	4.3E-02	5.6E-01	3.2E-01	7.0E-01	8.1E+00	9.4E-01	8.0E+00	1.8E+00		2.2E-01	7.3E+00
+f>	2.2E-02	1.1E-05	1.2E-02	3.6E-01	9.5E-02	1.5E-01	3.0E-02	1.0E-01	6.8E-01	4.4E-02	1.9E+00	3.2E-01	7.3E+00	2.2E-01		4.8E-02
-f>	1.1E-05	2.2E-02	3.6E-01	1.2E-02	1.5E-01	9.5E-02	1.0E-01	3.0E-02	4.4E-02	6.8E-01	3.2E-01	1.9E+00	2.2E-01	7.3E+00	4.8E-02	

Table S38. Average transition magnetic moment elements between the states of 5, given in  $\mu_B^2$ .

	$ +\frac{15}{2}>$	$ -\frac{15}{2}>$	+a>	-a>	+b>	-b>	+c>	-c>	+d>	-d>	+e>	-e>	+f>	-f>	+g>	-g>
$ +\frac{15}{2}>$		1.6E-08	4.3E+00	1.5E-06	1.1E-01	1.2E-03	3.9E-03	6.3E-04	7.5E-03	5.8E-03	7.7E-03	8.3E-03	2.4E-03	2.4E-04	7.2E-03	2.3E-05
$ -\frac{15}{2}>$	1.6E-08		1.5E-06	4.3E+00	1.2E-03	1.1E-01	6.3E-04	3.9E-03	5.8E-03	7.5E-03	8.3E-03	7.7E-03	2.4E-04	2.4E-03	2.3E-05	7.2E-03
+a>	4.3E+00	1.5E-06		3.3E-05	6.1E+00	7.5E-02	8.1E-01	2.2E-02	4.5E-01	2.5E-01	2.6E-01	2.0E-01	2.3E-01	9.5E-03	9.1E-02	4.1E-04
-a>	1.5E-06	4.3E+00	3.3E-05		7.5E-02	6.1E+00	2.2E-02	8.1E-01	2.5E-01	4.5E-01	2.0E-01	2.6E-01	9.5E-03	2.3E-01	4.1E-04	9.1E-02
+b>	1.1E-01	1.2E-03	6.1E+00	7.5E-02		7.1E-01	3.3E+00	4.9E-01	3.9E+00	2.5E+00	2.2E+00	3.6E-01	1.1E+00	1.3E-01	3.8E-01	6.9E-02
-b>	1.2E-03	1.1E-01	7.5E-02	6.1E+00	7.1E-01		4.9E-01	3.3E+00	2.5E+00	3.9E+00	3.6E-01	2.2E+00	1.3E-01	1.1E+00	6.9E-02	3.8E-01
+c>	3.9E-03	6.3E-04	8.1E-01	2.2E-02	3.3E+00	4.9E-01		6.7E+00	5.4E+00	1.4E+00	7.2E-01	1.5E+00	8.1E-01	3.0E-01	1.3E-01	1.6E-01
-c>	6.3E-04	3.9E-03	2.2E-02	8.1E-01	4.9E-01	3.3E+00	6.7E+00		1.4E+00	5.4E+00	1.5E+00	7.2E-01	3.0E-01	8.1E-01	1.6E-01	1.3E-01
+d>	7.5E-03	5.8E-03	4.5E-01	2.5E-01	3.9E+00	2.5E+00	5.4E+00	1.4E+00		6.6E+00	2.2E+00	1.7E+00	1.3E+00	1.9E+00	2.3E-01	1.9E-01
-d>	5.8E-03	7.5E-03	2.5E-01	4.5E-01	2.5E+00	3.9E+00	1.4E+00	5.4E+00	6.6E+00		1.7E+00	2.2E+00	1.9E+00	1.3E+00	1.9E-01	2.3E-01
+e>	7.7E-03	8.3E-03	2.6E-01	2.0E-01	2.2E+00	3.6E-01	7.2E-01	1.5E+00	2.2E+00	1.7E+00		9.1E+00	8.5E+00	4.3E+00	3.6E-01	7.0E-01
-e>	8.3E-03	7.7E-03	2.0E-01	2.6E-01	3.6E-01	2.2E+00	1.5E+00	7.2E-01	1.7E+00	2.2E+00	9.1E+00		4.3E+00	8.5E+00	7.0E-01	3.6E-01
+f>	2.4E-03	2.4E-04	2.3E-01	9.5E-03	1.1E+00	1.3E-01	8.1E-01	3.0E-01	1.3E+00	1.9E+00	8.5E+00	4.3E+00		5.3E+00	6.5E+00	1.2E+00
-f>	2.4E-04	2.4E-03	9.5E-03	2.3E-01	1.3E-01	1.1E+00	3.0E-01	8.1E-01	1.9E+00	1.3E+00	4.3E+00	8.5E+00	5.3E+00		1.2E+00	6.5E+00
+g>	7.2E-03	2.3E-05	9.1E-02	4.1E-04	3.8E-01	6.9E-02	1.3E-01	1.6E-01	2.3E-01	1.9E-01	3.6E-01	7.0E-01	6.5E+00	1.2E+00		3.3E-01
-g>	2.3E-05	7.2E-03	4.1E-04	9.1E-02	6.9E-02	3.8E-01	1.6E-01	1.3E-01	1.9E-01	2.3E-01	7.0E-01	3.6E-01	1.2E+00	6.5E+00	3.3E-01	

Table S39. Average transition magnetic moment elements between the states of 6, given in  $\mu_B^2$ .

	$ +\frac{15}{2}>$	$ -\frac{15}{2}>$	+a>	-a>	+b>	-b>	+c>	-c>	+d>	-d>	+e>	-e>	+f>	-f>	+g>	-g>
$ +\frac{15}{2}>$		5.8E-07	7.4E-03	1.1E+00	3.0E-02	1.3E-01	2.1E-02	4.2E-01	7.7E-02	7.7E-02	1.6E-01	3.7E-01	1.6E+00	4.7E-02	4.8E-01	3.0E-01
$ -\frac{15}{2}>$	5.8E-07		1.1E+00	7.4E-03	1.3E-01	3.0E-02	4.2E-01	2.1E-02	7.7E-02	7.7E-02	3.7E-01	1.6E-01	4.7E-02	1.6E+00	3.0E-01	4.8E-01
+a>	7.4E-03	1.1E+00		4.4E+00	8.3E+00	5.2E+00	6.1E+00	7.4E-01	1.6E+00	9.8E-01	9.7E-02	9.6E-01	8.8E-02	8.3E-01	1.2E-01	1.7E-01
-a>	1.1E+00	7.4E-03	4.4E+00		5.2E+00	8.3E+00	7.4E-01	6.1E+00	9.8E-01	1.6E+00	9.6E-01	9.7E-02	8.3E-01	8.8E-02	1.7E-01	1.2E-01
+b>	3.0E-02	1.3E-01	8.3E+00	5.2E+00		3.0E+00	3.1E+00	1.5E+00	5.7E+00	3.0E+00	5.7E-01	3.6E-01	5.7E-01	6.9E-01	1.0E-01	4.5E-01
-b>	1.3E-01	3.0E-02	5.2E+00	8.3E+00	3.0E+00		1.5E+00	3.1E+00	3.0E+00	5.7E+00	3.6E-01	5.7E-01	6.9E-01	5.7E-01	4.5E-01	1.0E-01
+c>	2.1E-02	4.2E-01	6.1E+00	7.4E-01	3.1E+00	1.5E+00		3.4E+00	2.0E+00	9.1E-01	5.5E+00	2.9E+00	2.2E-01	8.5E-01	1.3E+00	1.4E+00
-c>	4.2E-01	2.1E-02	7.4E-01	6.1E+00	1.5E+00	3.1E+00	3.4E+00		9.1E-01	2.0E+00	2.9E+00	5.5E+00	8.5E-01	2.2E-01	1.4E+00	1.3E+00
+d>	7.7E-02	7.7E-02	1.6E+00	9.8E-01	5.7E+00	3.0E+00	2.0E+00	9.1E-01		4.8E+00	5.3E+00	2.1E+00	1.2E+00	2.6E+00	3.6E-01	7.0E-01
-d>	7.7E-02	7.7E-02	9.8E-01	1.6E+00	3.0E+00	5.7E+00	9.1E-01	2.0E+00	4.8E+00		2.1E+00	5.3E+00	2.6E+00	1.2E+00	7.0E-01	3.6E-01
+e>	1.6E-01	3.7E-01	9.7E-02	9.6E-01	5.7E-01	3.6E-01	5.5E+00	2.9E+00	5.3E+00	2.1E+00		3.8E+00	3.2E+00	6.5E+00	2.9E+00	6.1E-01
-e>	3.7E-01	1.6E-01	9.6E-01	9.7E-02	3.6E-01	5.7E-01	2.9E+00	5.5E+00	2.1E+00	5.3E+00	3.8E+00		6.5E+00	3.2E+00	6.1E-01	2.9E+00
+f>	1.6E+00	4.7E-02	8.8E-02	8.3E-01	5.7E-01	6.9E-01	2.2E-01	8.5E-01	1.2E+00	2.6E+00	3.2E+00	6.5E+00		4.8E+00	6.1E+00	6.0E-01
-f>	4.7E-02	1.6E+00	8.3E-01	8.8E-02	6.9E-01	5.7E-01	8.5E-01	2.2E-01	2.6E+00	1.2E+00	6.5E+00	3.2E+00	4.8E+00		6.0E-01	6.1E+00
+g>	4.8E-01	3.0E-01	1.2E-01	1.7E-01	1.0E-01	4.5E-01	1.3E+00	1.4E+00	3.6E-01	7.0E-01	2.9E+00	6.1E-01	6.1E+00	6.0E-01		2.1E+01
-g>	3.0E-01	4.8E-01	1.7E-01	1.2E-01	4.5E-01	1.0E-01	1.4E+00	1.3E+00	7.0E-01	3.6E-01	6.1E-01	2.9E+00	6.0E-01	6.1E+00	2.1E+01	

Table S40. Average transition magnetic moment elements between the states of 7, given in  $\mu_B^2$ .

	$ +\frac{15}{2}>$	$ -\frac{15}{2}>$	+a>	-a>	+b>	-b>	+c>	-c>	+d>	-d>	+e>	-e>	+f>	-f>	+g>	-g>
$ +\frac{15}{2}>$		5.3E-09	4.3E-03	2.7E+00	2.4E-02	3.3E-02	1.1E+00	5.9E-02	2.4E-01	9.9E-02	2.0E-01	1.0E-01	5.1E-02	1.2E-02	1.3E-03	2.0E-03
$ -\frac{15}{2}>$	5.3E-09		2.7E+00	4.3E-03	3.3E-02	2.4E-02	5.9E-02	1.1E+00	9.9E-02	2.4E-01	1.0E-01	2.0E-01	1.2E-02	5.1E-02	2.0E-03	1.3E-03
+a>	4.3E-03	2.7E+00		2.2E-01	1.5E+01	5.9E-01	4.3E-01	1.5E+00	4.3E-01	3.6E-01	7.5E-02	4.1E-01	3.6E-02	4.5E-01	2.8E-03	1.0E-02
-a>	2.7E+00	4.3E-03	2.2E-01		5.9E-01	1.5E+01	1.5E+00	4.3E-01	3.6E-01	4.3E-01	4.1E-01	7.5E-02	4.5E-01	3.6E-02	1.0E-02	2.8E-03
+b>	2.4E-02	3.3E-02	1.5E+01	5.9E-01		1.3E+00	6.2E-01	1.1E+01	3.1E-01	1.2E+00	4.1E-01	3.0E-01	2.1E-01	7.2E-02	6.3E-02	3.0E-02
-b>	3.3E-02	2.4E-02	5.9E-01	1.5E+01	1.3E+00		1.1E+01	6.2E-01	1.2E+00	3.1E-01	3.0E-01	4.1E-01	7.2E-02	2.1E-01	3.0E-02	6.3E-02
+c>	1.1E+00	5.9E-02	4.3E-01	1.5E+00	6.2E-01	1.1E+01		4.9E+00	4.5E+00	7.9E+00	5.2E-01	2.1E-01	1.1E-01	7.8E-02	7.2E-02	3.8E-02
-c>	5.9E-02	1.1E+00	1.5E+00	4.3E-01	1.1E+01	6.2E-01	4.9E+00		7.9E+00	4.5E+00	2.1E-01	5.2E-01	7.8E-02	1.1E-01	3.8E-02	7.2E-02
+d>	2.4E-01	9.9E-02	4.3E-01	3.6E-01	3.1E-01	1.2E+00	4.5E+00	7.9E+00		4.8E+00	3.8E-01	5.8E-01	4.4E-01	1.9E-01	1.6E-02	1.4E-02
-d>	9.9E-02	2.4E-01	3.6E-01	4.3E-01	1.2E+00	3.1E-01	7.9E+00	4.5E+00	4.8E+00		5.8E-01	3.8E-01	1.9E-01	4.4E-01	1.4E-02	1.6E-02
+e>	2.0E-01	1.0E-01	7.5E-02	4.1E-01	4.1E-01	3.0E-01	5.2E-01	2.1E-01	3.8E-01	5.8E-01		1.6E+01	3.5E+00	3.7E+00	1.0E+00	5.7E-01
-e>	1.0E-01	2.0E-01	4.1E-01	7.5E-02	3.0E-01	4.1E-01	2.1E-01	5.2E-01	5.8E-01	3.8E-01	1.6E+01		3.7E+00	3.5E+00	5.7E-01	1.0E+00
+f>	5.1E-02	1.2E-02	3.6E-02	4.5E-01	2.1E-01	7.2E-02	1.1E-01	7.8E-02	4.4E-01	1.9E-01	3.5E+00	3.7E+00		1.6E+01	9.1E-01	2.5E+00
-f>	1.2E-02	5.1E-02	4.5E-01	3.6E-02	7.2E-02	2.1E-01	7.8E-02	1.1E-01	1.9E-01	4.4E-01	3.7E+00	3.5E+00	1.6E+01		2.5E+00	9.1E-01
+g>	1.3E-03	2.0E-03	2.8E-03	1.0E-02	6.3E-02	3.0E-02	7.2E-02	3.8E-02	1.6E-02	1.4E-02	1.0E+00	5.7E-01	9.1E-01	2.5E+00		1.9E+01
-g>	2.0E-03	1.3E-03	1.0E-02	2.8E-03	3.0E-02	6.3E-02	3.8E-02	7.2E-02	1.4E-02	1.6E-02	5.7E-01	1.0E+00	2.5E+00	9.1E-01	1.9E+01	

Table S41. Average transition magnetic moment elements between the states of 8, given in  $\mu_B^2$ .

	$ +\frac{15}{2}>$	$ -\frac{15}{2}>$	+a>	-a>	+b>	-b>	+c>	-c>	+d>	-d>	+e>	-e>	+f>	-f>	+g>	-g>
$ +\frac{15}{2}>$		5.6E-08	7.1E-03	2.0E+00	3.5E-02	4.5E-02	3.6E-02	1.3E+00	3.0E-01	1.9E-01	9.9E-02	2.6E-01	3.7E-01	1.1E-02	1.8E-02	9.6E-03
$ -\frac{15}{2}>$	5.6E-08		2.0E+00	7.1E-03	4.5E-02	3.5E-02	1.3E+00	3.6E-02	1.9E-01	3.0E-01	2.6E-01	9.9E-02	1.1E-02	3.7E-01	9.6E-03	1.8E-02
+a>	7.1E-03	2.0E+00		1.1E+00	2.0E+00	1.4E+01	1.4E+00	7.0E-01	1.3E+00	1.6E+00	1.2E-01	4.2E-01	4.1E-02	7.7E-01	3.7E-03	4.4E-02
-a>	2.0E+00	7.1E-03	1.1E+00		1.4E+01	2.0E+00	7.0E-01	1.4E+00	1.6E+00	1.3E+00	4.2E-01	1.2E-01	7.7E-01	4.1E-02	4.4E-02	3.7E-03
+b>	3.5E-02	4.5E-02	2.0E+00	1.4E+01		4.7E+00	2.1E+00	6.4E+00	9.0E-01	6.8E-01	2.5E-01	1.3E+00	5.5E-01	3.9E-01	1.3E-01	1.3E-01
-b>	4.5E-02	3.5E-02	1.4E+01	2.0E+00	4.7E+00		6.4E+00	2.1E+00	6.8E-01	9.0E-01	1.3E+00	2.5E-01	3.9E-01	5.5E-01	1.3E-01	1.3E-01
+c>	3.6E-02	1.3E+00	1.4E+00	7.0E-01	2.1E+00	6.4E+00		5.6E+00	3.9E+00	6.3E+00	4.9E-01	7.5E-01	3.6E-02	1.3E+00	1.3E-01	1.7E-01
-c>	1.3E+00	3.6E-02	7.0E-01	1.4E+00	6.4E+00	2.1E+00	5.6E+00		6.3E+00	3.9E+00	7.5E-01	4.9E-01	1.3E+00	3.6E-02	1.7E-01	1.3E-01
+d>	3.0E-01	1.9E-01	1.3E+00	1.6E+00	9.0E-01	6.8E-01	3.9E+00	6.3E+00		5.8E+00	3.1E+00	5.6E+00	9.9E-01	2.9E+00	4.0E-02	9.4E-02
-d>	1.9E-01	3.0E-01	1.6E+00	1.3E+00	6.8E-01	9.0E-01	6.3E+00	3.9E+00	5.8E+00		5.6E+00	3.1E+00	2.9E+00	9.9E-01	9.4E-02	4.0E-02
+e>	9.9E-02	2.6E-01	1.2E-01	4.2E-01	2.5E-01	1.3E+00	4.9E-01	7.5E-01	3.1E+00	5.6E+00		1.1E+01	1.9E+00	2.5E+00	3.7E+00	1.6E+00
-e>	2.6E-01	9.9E-02	4.2E-01	1.2E-01	1.3E+00	2.5E-01	7.5E-01	4.9E-01	5.6E+00	3.1E+00	1.1E+01		2.5E+00	1.9E+00	1.6E+00	3.7E+00
+f>	3.7E-01	1.1E-02	4.1E-02	7.7E-01	5.5E-01	3.9E-01	3.6E-02	1.3E+00	9.9E-01	2.9E+00	1.9E+00	2.5E+00		6.6E+00	7.5E-01	6.8E-01
-f>	1.1E-02	3.7E-01	7.7E-01	4.1E-02	3.9E-01	5.5E-01	1.3E+00	3.6E-02	2.9E+00	9.9E-01	2.5E+00	1.9E+00	6.6E+00		6.8E-01	7.5E-01
+g>	1.8E-02	9.6E-03	3.7E-03	4.4E-02	1.3E-01	1.3E-01	1.3E-01	1.7E-01	4.0E-02	9.4E-02	3.7E+00	1.6E+00	7.5E-01	6.8E-01		3.0E+01
-g>	9.6E-03	1.8E-02	4.4E-02	3.7E-03	1.3E-01	1.3E-01	1.7E-01	1.3E-01	9.4E-02	4.0E-02	1.6E+00	3.7E+00	6.8E-01	7.5E-01	3.0E+01	

Table S42. Average transition magnetic moment elements between the states of 9, given in  $\mu_B^2$ .

	$ +\frac{15}{2}>$	$ -\frac{15}{2}>$	+a>	-a>	+b>	-b>	+c>	-c>	+d>	-d>	+e>	-e>	+f>	-f>	+g>	-g>
$ +\frac{15}{2}>$		3.8E-08	1.3E+00	1.0E-03	5.9E-02	8.5E-03	1.1E+00	2.2E-01	7.3E-01	2.6E-01	1.3E-01	4.1E-01	4.1E-01	1.2E-02	1.4E-02	1.3E-02
$ -\frac{15}{2}>$	3.8E-08		1.0E-03	1.3E+00	8.5E-03	5.9E-02	2.2E-01	1.1E+00	2.6E-01	7.3E-01	4.1E-01	1.3E-01	1.2E-02	4.1E-01	1.3E-02	1.4E-02
+a>	1.3E+00	1.0E-03		5.3E-01	1.5E+01	5.6E-01	1.7E+00	1.8E+00	6.6E-01	1.3E+00	3.9E-01	1.1E-01	4.7E-01	3.6E-02	2.8E-02	9.1E-03
-a>	1.0E-03	1.3E+00	5.3E-01		5.6E-01	1.5E+01	1.8E+00	1.7E+00	1.3E+00	6.6E-01	1.1E-01	3.9E-01	3.6E-02	4.7E-01	9.1E-03	2.8E-02
+b>	5.9E-02	8.5E-03	1.5E+01	5.6E-01		1.4E+00	5.0E+00	1.7E+00	2.7E-01	6.6E-01	2.4E-01	4.7E-01	5.1E-01	6.5E-02	7.5E-02	1.4E-01
-b>	8.5E-03	5.9E-02	5.6E-01	1.5E+01	1.4E+00		1.7E+00	5.0E+00	6.6E-01	2.7E-01	4.7E-01	2.4E-01	6.5E-02	5.1E-01	1.4E-01	7.5E-02
+c>	1.1E+00	2.2E-01	1.7E+00	1.8E+00	5.0E+00	1.7E+00		1.0E+01	8.2E+00	2.5E+00	5.5E-01	5.5E-01	7.4E-01	3.3E-01	1.6E-01	1.4E-01
-c>	2.2E-01	1.1E+00	1.8E+00	1.7E+00	1.7E+00	5.0E+00	1.0E+01		2.5E+00	8.2E+00	5.5E-01	5.5E-01	3.3E-01	7.4E-01	1.4E-01	1.6E-01
+d>	7.3E-01	2.6E-01	6.6E-01	1.3E+00	2.7E-01	6.6E-01	8.2E+00	2.5E+00		4.2E+00	2.2E+00	7.4E+00	5.4E-01	2.9E+00	4.0E-02	6.0E-02
-d>	2.6E-01	7.3E-01	1.3E+00	6.6E-01	6.6E-01	2.7E-01	2.5E+00	8.2E+00	4.2E+00		7.4E+00	2.2E+00	2.9E+00	5.4E-01	6.0E-02	4.0E-02
+e>	1.3E-01	4.1E-01	3.9E-01	1.1E-01	2.4E-01	4.7E-01	5.5E-01	5.5E-01	2.2E+00	7.4E+00		7.4E+00	2.3E+00	2.5E+00	1.8E+00	2.8E+00
-e>	4.1E-01	1.3E-01	1.1E-01	3.9E-01	4.7E-01	2.4E-01	5.5E-01	5.5E-01	7.4E+00	2.2E+00	7.4E+00		2.5E+00	2.3E+00	2.8E+00	1.8E+00
+f>	4.1E-01	1.2E-02	4.7E-01	3.6E-02	5.1E-01	6.5E-02	7.4E-01	3.3E-01	5.4E-01	2.9E+00	2.3E+00	2.5E+00		6.0E+00	5.0E-01	8.4E-01
-f>	1.2E-02	4.1E-01	3.6E-02	4.7E-01	6.5E-02	5.1E-01	3.3E-01	7.4E-01	2.9E+00	5.4E-01	2.5E+00	2.3E+00	6.0E+00		8.4E-01	5.0E-01
+g>	1.4E-02	1.3E-02	2.8E-02	9.1E-03	7.5E-02	1.4E-01	1.6E-01	1.4E-01	4.0E-02	6.0E-02	1.8E+00	2.8E+00	5.0E-01	8.4E-01		2.5E+01
-g>	1.3E-02	1.4E-02	9.1E-03	2.8E-02	1.4E-01	7.5E-02	1.4E-01	1.6E-01	6.0E-02	4.0E-02	2.8E+00	1.8E+00	8.4E-01	5.0E-01	2.5E+01	

Table S43. Average transition magnetic moment elements between the states of 10, given in  $\mu_B^2$ .