# **ELECTRONIC SUPPORTING INFORMATION**

# Slow magnetic dynamics in a family of mononuclear lanthanide complexes

# exhibiting the rare cubic coordination geometry

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### Synthesis

All syntheses were performed under ambient conditions.  $Co(dbm)_2^1$  and  $KTp^2$  were synthesized according to published procedures. All other chemicals were commercially available and used as received.

**Synthesis of**  $[Co^{III}(Tp)_2]_{1.3}[Tb(NO_3)_2(dbm)_2](NO_3)_{0.3}$  (1). To a colorless solution of KTp (12.6 mg, 0.05 mmol) in MeCN (7.5 mL) was added solid Co(dbm)<sub>2</sub> (25.2 mg, 0.05 mmol) followed by stirring for 5 min. The reagent Tb(NO<sub>3</sub>)<sub>3</sub>·5H<sub>2</sub>O (21.7 mg, 0.05 mmol) was then added and the resulting dark orange solution was stirred for a further 15 min. The solution was subsequently filtered, and left undisturbed for crystallization. Slow evaporation of the solvent gave diffraction quality crystals of 1 after 1 week which were collected by filtration, washed with hexanes (3 x 5 mL) and dried in air. Yield is 65% (45.69 mg). Anal. Calc. for C<sub>54</sub>H<sub>48.67</sub>N<sub>18.33</sub>B<sub>2.67</sub>O<sub>11</sub>Co<sub>1.33</sub>Tb (1): C, 46.44; H, 3.51; N, 18.38 %. Found: C, 46.55; H, 3.57; N, 18.28 %. Selected ATR data (Nujol mull, cm<sup>-1</sup>): 1589 (w), 1541 (w), 1516 (w), 1305 (s), 1221 (m), 1117 (m), 1073 (m), 1053 (m), 800 (w), 771 (m), 721 (s), 681 (m), 617 (w), 511 (w).

**Synthesis of**  $[Co^{III}(Tp)_2]_{1.3}[Dy(NO_3)_2(dbm)_2](NO_3)_{0.3}$  (2). This complex was prepared in the same manner as complex 1 but using Dy(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O (22.8 mg, 0.05 mmol) in place of Tb(NO<sub>3</sub>)<sub>3</sub>·5H<sub>2</sub>O. After 1 week, diffraction quality crystals of 2 had appeared; these were collected by filtration and washed with Hexanes (3 x 5 mL); the yield is 55% (38.50 mg). Anal. Calc. for C<sub>54</sub>H<sub>48.67</sub>N<sub>18.33</sub>B<sub>2.67</sub>O<sub>11</sub>Co<sub>1.33</sub>Dy (2): C, 46.32; H, 3.50; N, 18.34 %. Found: C, 46.23; H, 3.37; N, 18.21 %. Selected ATR data (Nujol mull, cm<sup>-1</sup>): 1589 (m), 1542 (m), 1516 (w), 1323 (m), 1220 (m), 1118 (m), 1073 (m), 1053 (m), 772 (m), 745 (s), 721 (s), 682 (m), 619 (w), 509 (w).

**Synthesis of**  $[Co^{III}(Tp)_2]_{1.3}[Er(NO_3)_2(dbm)_2](NO_3)_{0.3}$  (3). This complex was prepared in the same manner as complex 1 but using  $Er(NO_3)_3 \cdot 5H_2O$  (22.1 mg, 0.05 mmol) in place of Tb(NO<sub>3</sub>)\_3 \cdot 5H\_2O. After 1 week, diffraction quality crystals of **3** had appeared; these were collected by filtration and washed with hexanes (3 x 5 mL); the yield is 60% (42.14 mg). Anal. Calc. for  $C_{54}H_{48.67}N_{18.33}B_{2.67}O_{11}Co_{1.33}Er$  (**3**): C, 46.17; H, 3.49; N, 18.27 %. Found: C, 46.28; H, 3.57; N, 18.19 %. Selected ATR data (Nujol mull, cm<sup>-1</sup>): 1587 (w), 1540 (w), 1516 (w), 1305 (m), 1221 (m), 1117 (m), 1075 (m), 1053 (m), 774 (m), 742 (m), 722 (m), 681 (w), 620 (w).

**Synthesis of**  $[Co^{III}(Tp)_2]_{1.3}[Y(NO_3)_2(dbm)_2](NO_3)_{0.3}$  (4). This complex was prepared in the same manner as complex 1 but using  $Y(NO_3)_3$ ·6H<sub>2</sub>O (21.7 mg, 0.05 mmol) in place of Tb(NO<sub>3</sub>)<sub>3</sub>·5H<sub>2</sub>O. After 1 week, diffraction quality crystals of 4 had appeared which were collected by filtration and washed with hexanes (3 x 5 mL); the yield is 50% (33.16 mg). Anal. Calc. for C<sub>54</sub>H<sub>48.67</sub>N<sub>18.33</sub>B<sub>2.67</sub>O<sub>11</sub>Co<sub>1.33</sub>Y (4): C, 48.89; H, 3.70; N, 19.35 %. Found: C, 49.01; H, 3.59; N, 19.27 %. Selected ATR data (Nujol mull, cm<sup>-1</sup>): 1590 (m), 1543 (s), 1516 (m), 1306 (m), 1221 (m), 1117 (m), 1072 (m), 1053 (m), 938 (m), 800 (w), 771 (m), 744 (s), 721 (s), 681 (m), 659 (w), 617 (w), 514 (w).

### X-ray Crystallography

Structural characterization of the complexes was performed on single crystals at the APS housed in the Argonne National Laboratory. X-ray data were collected using a synchrotron source with a wavelength of 0.41328 Å and a Pilatus 1M (CdTe) pixel array detector. Crystals suitable for diffraction were affixed to glass fibers using ®Paratone oil. Collection was performed at 100 K under a N<sub>2</sub> cold stream. The frames were integrated using the Apex II software program with a pre-existing mask supplied before collection.<sup>3</sup> A multiscan absorption correction was performed using SADABS within the APEX II software suite. The structures were solved with SHELXT<sup>4</sup> and refined with SHELXL-2014<sup>5</sup> within the OLEX program.<sup>6</sup> Dispersion corrections calculated in PLATON were applied to all structures for each element according to the wavelength of collection.<sup>7</sup> All hydrogen atoms were placed in calculated positions. All non-hydrogen atoms were finished with anisotropic refinement.

The structures for  $[Co^{III}(Tp)_2]_{1.3}[Tb(NO_3)_2(dbm)_2](NO_3)_{0.3}$ ,  $[Co^{III}(Tp)_2]_{1.3}[Dy(NO_3)_2(dbm)_2](NO_3)_{0.3}$ ,  $[Co^{III}(Tp)_2]_{1.3}[Er(NO_3)_2(dbm)_2](NO_3)_{0.3}$ , and  $[Co^{III}(Tp)_2]_{1.3}[Y(NO_3)_2(dbm)_2](NO_3)_{0.3}$  were all refined in the cubic space group *I*23 as an inversion twin with minor components of 0.49, 0.42, 0.45, and 0.47 for the Tb, Dy, Er, and Y complexes respectively. The higher symmetry space group Im-3 was investigated but the additional mirror plane symmetry does not allow for torsion in the bidentate ligands coordinated to the lanthanide metal centers. In order to obtain a more accurate model of these ligands, the structure was refined as an inversion twin in the lower symmetry space group. Each of the structures was run through the program SQUEEZE.<sup>8</sup> The electron density accounts for the remaining 1/3 of a nitrate anion needed to charge balance the compound as well as cocrystallizing acetonitrile molecules. Attempts were made to try and model the disorder but were not successful. The electron density after accounting for the nitrate anion results in 5.3, 4.3, 5.1, and 4.4 acetonitrile molecules in the Tb, Dy, Er, and Y complexes respectively.

There is a small amount of disorder in the lanthanide metal centers and directly coordinated atoms. Modeling this disorder did not significantly improve the refinement. The Cambridge Crystallographic Database Centre numbers for each complex are: 1847190 for  $[Co^{III}(Tp)_2]_{1.3}[Tb(NO_3)_2(dbm)_2](NO_3)_{0.3}$ , 1847187 for  $[Co^{III}(Tp)_2]_{1.3}[Dy(NO_3)_2(dbm)_2](NO_3)_{0.3}$ , 1847188 for  $[Co^{III}(Tp)_2]_{1.3}[Er(NO_3)_2(dbm)_2](NO_3)_2(dbm)_2](NO_3)_{0.3}$ , and 1847189 for  $[Co^{III}(Tp)_2]_{1.3}[Y(NO_3)_2(dbm)_2](NO_3)_{0.3}$ . Unit cell parameters, structure solution and refinement details for all complexes are summarized in Table S1. Further crystallographic details can be found in the corresponding CIF files provided in the Supporting Information. The programs used for molecular graphics were MERCURY<sup>9</sup> and Diamond.<sup>10</sup>

Complex	1	2	3	4
Empirical formula	$C_{54}H_{48.67}B_{2.67}Co_{1.33}N_{18}O_{10}Tb$	C <sub>54</sub> H <sub>48.67</sub> B <sub>2.67</sub> Co <sub>1.33</sub> N <sub>18</sub> O <sub>10</sub> Dy	r C <sub>54</sub> H <sub>48.67</sub> B <sub>2.67</sub> Co <sub>1.33</sub> N <sub>18</sub> O <sub>10</sub> Er	C <sub>54</sub> H <sub>48.67</sub> B <sub>2.67</sub> Co <sub>1.33</sub> N <sub>18</sub> O <sub>10</sub> Y
Formula weight	1376.08	1379.67	1384.44	1306.08
Temperature/K	100.0	100.0	100.0	100.0
Crystal system	cubic	cubic	cubic	cubic
Space group	I23	123	123	123
a/Å	20.9135(4)	20.9059(3)	20.9076(4)	20.9091(4)
b/Å	20.9135(4)	20.9059(3)	20.9076(4)	20.9091(4)
c/Å	20.9135(4)	20.9059(3)	20.9076(4)	20.9091(4)
a/°	90	90	90	90
β/°	90	90	90	90
γ/°	90	90	90	90
Volume/Å <sup>3</sup>	9147.0(5)	9137.1(4)	9139.3(5)	9141.3(5)
Z	6	6	6	6
$\rho_{calc}g/cm^3$	1.499	1.504	1.509	1.424
µ/mm <sup>-1</sup>	0.396	0.397	0.434	0.338
F(000)	4158.0	4164.0	4176.0	4002.0
Crystal size/mm <sup>3</sup>	$0.94 \times 0.121 \times 0.113$	$0.143 \times 0.13 \times 0.071$	$0.255 \times 0.242 \times 0.214$	$0.97 \times 0.105 \times 0.102$
	Synchrotron	Synchrotron	Synchrotron	Synchrotron
Radiation	$(\lambda = 0.41328)$	$(\lambda = 0.41328)$	$(\lambda = 0.41328)$	$(\lambda = 0.41328)$
20 range for data collection/°	2.774 to 30.706	2.774 to 40.22	2.774 to 40.356	2.774 to 35.354
	$-18 \le h \le 18$	$-24 \leq h \leq 24$	$-24 \leq h \leq 24$	$-21 \le h \le 21$
Index ranges	$0 \le k \le 18$	$0 \leq k \leq 24$	$0 \leq k \leq 24$	$0 \leq k \leq 21$
	$2 \le l \le 26$	$2 \le l \le 34$	$2 \leq l \leq 34$	$2 \leq l \leq 30$
Reflections collected	3381	7378	7435	5076
	3381	7378	7435	5076
Independent reflections	$R_{int} = 0.0442$	$R_{int} = 0.0392$	$R_{int} = 0.0431$	$R_{int} = 0.0413$
	$R_{sigma} = 0.0105$	$R_{sigma} = 0.0116$	$R_{sigma} = 0.0120$	$R_{sigma} = 0.0117$
Data/restraints/ parameters	3381 / 0 / 200	7378 / 0 / 200	7435 / 0 / 200	5076 / 0 / 200
Goodness-of-fit on F <sup>2</sup>	1.147	1.076	1.064	1.063
Final R <sup><i>a,b</i></sup> indexes	$R_1 = 0.0334$	$R_1 = 0.0469$	$R_1 = 0.0454$	$R_1 = 0.0330$
[I>=2σ (I)]	$wR_2 = 0.0810$	$wR_2 = 0.1192$	$wR_2 = 0.1191$	$wR_2 = 0.0890$
Final R a,b indexes	$R_1 = 0.0337$	$R_1 = 0.0505$	$R_1 = 0.0474$	$R_1 = 0.0348$
[all data]	$wR_2 = 0.0813$	$wR_2 = 0.1217$	$wR_2 = 0.1208$	$wR_2 = 0.0901$
Largest diff. peak /hole / e Å <sup>-3</sup>	0.40 / -1.36	1.64 / -3.50	1.70 / -3.76	0.37 / -1.25

 Table S1. Crystal data and structural refinement parameters for compounds 1-4.

 $\overline{{}^{a}\mathbf{R}_{1} = \Sigma(||F_{o}| - |F_{c}||)/\Sigma|F_{o}|}. \ {}^{b}\mathbf{w}\mathbf{R}_{2} = [\Sigma[w(F_{o}^{2} - F_{c}^{2})^{2}]/\Sigma[w(F_{o}^{2})^{2}]]^{1/2}, w = 1/[\sigma^{2}(F_{o}^{2}) + (ap)^{2} + bp],$ 

where  $p = [\max(F_0^2, 0) + 2F_c^2]/3$ .







Figure S1. Experimental and theoretical powder-XRD patterns for complexes 1-4.



**Figure S2**. Molecular structure of **2**. Color scheme: Dy, yellow; Co<sup>III</sup>, green; N, blue; O, red; B, pink; C, black. Hydrogen atoms are omitted for sake of clarity.



Figure S3. Packing diagram of 2 along  $\alpha$  axis. Hydrogen atoms are omitted for the sake of clarity.

**Table S2.** Shape measures of the 8-coordinate lanthanide coordination polyhedra. The values in boldface indicate the closest polyhedron according to the Continuous Shape Measures.

 Polyhedron <sup>c</sup>	Tb1	Dv1	Er1	Y1
 OP-8	31.30	31.80	31.00	31.48
HPY-8	26.19	26.23	26.28	26.27
HBPY-8	7.88	7.78	8.18	7.96
CU-8	3.26	3.07	3.60	3.37
SAPR-8	6.83	6.97	5.83	6.34
TDD-8	5.97	6.02	5.29	5.61
JGBF-8	11.07	11.22	10.81	10.93
JETBPY-8	22.39	22.29	22.66	22.45
JBTPR-8	7.15	7.31	6.17	6.65
BTPR-8	7.05	7.23	6.06	6.56
JSD-8	8.18	8.38	7.10	7.61
TT-8	4.18	3.99	4.51	4.29
ETBPY-8	20.68	20.67	20.91	20.75

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

Compound <sup>d</sup>	1	3	4
$d_{M-O1}$ / Å	2.280(1)	2.253(2)	2.259(1)
$d_{M\text{-}O2} \ / \ \mathring{A}$	2.499(2)	2.461(1)	2.478(1)
$d_{M-Oplane}$ / Å	1.183(2)	1.184(2)	1.188(2)
$d_{pp}$ / Å	2.367(2)	2.368(2)	2.375(2)
$d_{in}$ / Å	2.908(2)	2.862(1)	2.876(1)
φ / °	13.46	16.49	14.93
θ/°	59.84	59.36	59.40

**Table S3.** Key geometrical parameters analyzed for the coordination environment of 8coordinate lanthanide ions in 1, 3, and 4.

<sup>*d*</sup> Abbreviations:  $d_{M-O1}$  and  $d_{M-O2}$ , metal-oxygen distances;  $d_{M-Oplane}$ , distance between the metal ion and the O<sub>4</sub>-plane;  $d_{pp}$ , distance between the upper and lower O<sub>4</sub>-planes;  $d_{in}$ , the shortest O-O distance in the O<sub>4</sub>-plane;  $\phi$ , skew or twist angle, angle between the diagonals of the two different O<sub>4</sub>-planes (average value);  $\theta$ , compression angle, angle between the four-fold axis and the M-O bond direction.

Compound	1	2	3	4	
Co <sup>II</sup>	3.43	3.47	3.46	3.46	
Co <sup>III</sup>	<u>3.17</u>	<u>3.20</u>	<u>3.19</u>	<u>3.19</u>	

Table S4. Bond valence sum (BVS)<sup>e</sup> calculations for Co atoms in 1-4.

<sup>*e*</sup> The underlined value is the one closest to the charge for which it was calculated. The oxidation state is the nearest whole number to the underlined value.

# Magnetism



Figure S4. Magnetization (M) vs field (H) plot for complex 1 at 2 K.



Figure S5. Magnetization (M) vs field (H) plot for complex 2 at 2 K.



Figure S6. Magnetization (M) vs field (H) plot for complex 3 at 2 K.



**Figure S7.** Plot of reduced magnetization  $(M/N\mu_B)$  vs. HT<sup>-1</sup> for compound **1** at applied fields of 2–7 T and in the 2–5 K temperature range. Solid lines are guides for the eye.



**Figure S8.** Plot of reduced magnetization (M/N $\mu_B$ ) vs. HT<sup>-1</sup> for compound **2** at applied fields of 2–7 T and in the 2–5 K temperature range. Solid lines are guides for the eye.



**Figure S9.** Plot of reduced magnetization (M/N $\mu_B$ ) vs. HT<sup>-1</sup> for compound **3** at applied fields of 2–7 T and in the 2–5 K temperature range. Solid lines are guides for the eye.



**Figure S10**. Out-of-phase susceptibility for **1** in various applied DC fields at 1.8 K. Solid lines are guides for the eye.



Figure S11. Out-of-phase susceptibility for 2 in various applied DC fields at 1.8 K. Solid lines are guide for the eye.



Figure S12. Out-of-phase susceptibility for 2 in various applied DC fields at 10 K. Solid lines are guide for the eye.



**Figure S13**. Out-of-phase susceptibility for **3** in various applied DC fields at 1.8 K. Solid lines are guides for the eye.



**Figure S14**. Temperature dependence of the in-phase  $\chi'T$  product (top) and out-of-phase  $\chi''$  (bottom) ac susceptibility signals of **2** in a 2.0 G field oscillating at the indicated frequencies.



**Figure S15**. In-phase ( $\chi'$ ) component of the magnetic susceptibility vs. frequency, under a 0.02 T applied *dc* field, for complex **2**. Solid lines are guides for the eye.



**Figure S16**. Cole-Cole plot for **2** obtained using the ac susceptibility data in 0.02 T applied *dc* field. The solid lines correspond to the best fit obtained with a generalized Debye model.



**Figure S17**. Magnetization (M) vs. applied dc field (H) measurements for a microcrystalline sample of **2** at 1.8 K.

**Table S5.** Cole-Cole fit values of **2** between 2-19 K under an applied *dc* field of 0.02 T and an *ac*field of 2.0 Oe.

T / K	$\chi_S$ / cm <sup>3</sup> mol <sup>-1</sup>	$\chi_{t1}$ / cm <sup>3</sup> mol <sup>-1</sup>	$\tau_1 / s$	$\alpha_1$	$\chi_{t2}$ / cm <sup>3</sup> mol <sup>-1</sup>	$\tau_2 / s$	$\alpha_2$	Residual
2	0.55069	3.13848	0.00002	0.27804	2.33314	0.06064	0.23378	0.00659
3	0.00000	3.22751	0.00003	0.25272	1.26539	0.03204	0.21237	0.00241
4	0.00000	1.90703	0.00000	0.24726	1.28006	0.01870	0.30565	0.00176
5	0.00000	1.51655	0.00000	0.24297	1.02052	0.01025	0.25983	0.00481
6	0.00000	1.25676	0.00000	0.24068	0.83229	0.00550	0.19057	0.00582
7	0.00001	1.06404	0.00000	0.23550	0.71464	0.00302	0.14346	0.00349
8	0.00002	0.92176	0.00001	0.23449	0.62642	0.00175	0.10450	0.00177
9	0.00002	0.82021	0.00001	0.22354	0.55522	0.00108	0.07779	0.00058
10	0.00004	0.75121	0.00001	0.21271	0.48691	0.00072	0.05244	0.00020

11	0.00007	0.70377	0.00001	0.20999	0.42295	0.00051	0.03227	0.00014
12	0.00016	0.63792	0.00001	0.00000	0.39710	0.00036	0.03381	0.00011
13	0.00037	0.62004	0.00001	0.00000	0.33656	0.00028	0.01839	0.00010
14	0.00122	0.60764	0.00001	0.00000	0.28173	0.00022	0.00970	0.00008
15	0.00159	0.60196	0.00001	0.00000	0.22932	0.00019	0.00813	0.00007
16	0.00664	0.60369	0.00001	0.00000	0.17156	0.00016	0.00000	0.00008
17	0.00663	0.61450	0.00002	0.00000	0.11608	0.00015	0.00000	0.00007
18	0.00466	0.62991	0.00002	0.00000	0.06346	0.00016	0.00000	0.00006
19	0.00422	0.62789	0.00002	0.00000	0.03075	0.00018	0.00000	0.00005
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### **Computational Details**

#### Ab initio calculations

Using MOLCAS 8.0,<sup>11</sup> *ab initio* calculations were performed for the Dy<sup>III</sup> ion using the crystal structures of **2** to rationalize the observed SMM behavior. Relativistic effects are taken into account on the basis of the Douglas–Kroll Hamiltonian.<sup>12</sup> The spin-free eigen states are achieved by the Complete Active Space Self-Consistent Field (CASSCF) method.<sup>13</sup> The basis sets were taken from the ANORCC library for the calculations.<sup>14</sup> We employed the [ANO-RCC... 8s7p5d3f2g1h.] basis set for Dy<sup>III</sup> atoms, the [ANO-RCC...3s2p.] basis set for C atoms, the [ANO-RCC...2s.] basis set for H atoms, the [ANO-RCC...3s2p1d.] basis set for N atoms, and the [ANO-RCC...3s2p1d.] basis set for O atoms. In the first step, a guessorb calculation was run using Seward module to create the starting guess orbitals. Nine electrons across seven 4f orbitals of the Dy<sup>III</sup> ion were included. Then using these guess orbitals, we chose the active space based on the number of active electrons in the number of active orbitals and carried out the SA-CASSCF calculations. The Configuration Interaction (CI) procedure was computed for Dy<sup>III</sup> ion and considered twenty-one sextet excited states in the calculations to compute the anisotropy.

After computing these excited states, the RASSI-SO<sup>15</sup> module was used to calculate the spinorbit (SO) coupled states. Moreover, these computed SO states were considered in the SINGLE\_ANISO<sup>16</sup> program to compute the *g*-tensors. The *g*-tensors for the Kramers doublets of  $Dy^{3+}$  were computed based on the pseudospin S =  $\frac{1}{2}$  formalism.<sup>16</sup> Crystal-field (CF) parameters were extracted using the SINGLE\_ANISO code, as implemented in MOLCAS 8.0.

**Table S6.** *Ab Initio* Computed Eight Low-lying Kramers Doublet Energies (cm<sup>-1</sup>) and g-tensors of each Kramers Doublets in **2**.

KDs	Energy (cm <sup>-1</sup> )	$g_x$ , $g_y$ and $g_z$
1	0.0	0.0202
		0.0237
		19.7199
2	234.9	0.0459
		0.1109
		15.4744
3	317.6	1.8979
		2.0641
		12.2892
4	457.0	1.7856
		4.3905
		9.4439
5	572.6	0.1305
		1.2204
		17.9329
6	609.6	8.1826
		8.0311
		0.0825
7	716.1	3.5694
		4.1807
		12.2314
8	886.1	0.3676
		0.6645
		18.3199

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