Supplementary Materials: Magneto-Luminescence Correlation in the Textbook Dysprosium(III) Nitrate Single-Ion Magnet

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Table S1. Crystal and structure refinement data for compound **1**.

Compound	1
Formula	$DyH_{12}N_3O_{15}$
Formula weight	456.60
Temperature/K	293
Crystal system	Triclinic
Space group	*P*-1
a/Å	6.7429(8)
b/Å	9.1094(9)
c/Å	11.6502(11)
α/°	70.369(9)
β/°	88.714(9)
γ/°	69.113(11)
Volume/Å^3	625.86(13)
Z	2
Dc/g·cm^{-3}	2.4228
μ(Mo-Kα)/mm^{-1}	6.054
F(000)	414.2
Crystal size/mm	0.1 × 0.1 × 0.1
Crystal type	Colourless plates
θ range	3.25 to 29.29
Index ranges	$-9 \le h \le 9$ $-12 \le k \le 11$ $-14 \le l \le 14$
Reflections collected	5351
Independent reflections	2879 (R_{int} = 0.0424)
Data/parameters	2879/171
Final *R* indices [$I > 2\sigma(I)$][a,b]	R_1 = 0.0369 wR_2 = 0.0765
Final *R* indices (all data)[a,b]	R_1 = 0.0443 wR_2 = 0.0848
Largest diff. peak and hole	1.18 and −1.64 eÅ^{-3}

[a] $R_1 = \sum \left| |F_o| - |F_c| \right| / \sum |F_o|$; [b] $wR_2 = \sqrt{\sum \left[w\left(F_o^2 - F_c^2\right)^2 \right] / \sum \left[w\left(F_o^2\right)^2 \right]}$

Table S2. SHAPE analysis for compound **1**.

DP	EPY	OBPY	PPR	PAPR	JBCCU	JPCSAPR	JMBIC	JATDI	JSPC	SDD	TD	HD
33.818	23.117	17.902	9.556	14.372	11.933	4.385	8.791	17.518	2.204	6.675	6.077	10.278

DP, decagon; EPY, ennegonal pyramid; OBPY, octagonal pyramid; PPR, pentagonal prism; PAPR, pentagonal antiprism; JBCCU, bicapped cube; JPCSPAR, bicapped square antiprism; JMBIC, metabidiminished icosahedron; JATDI, augmented tridiminished icosahedron; JSPC, spherocorona; SDD, staggered dodecahedron; TD, tetradecahedron; HD, hexadecahedron.

Table S3. Fitting of the Cole–Cole plots with a generalized Debye model for temperature ranging from 1.8 to 4.1 K under a 2000 Oe DC field for **1**.

T (K)	α	χ_S (cm³·mol⁻¹)	χ_T (cm³·mol⁻¹)
3.750	0.145	0.436	1.803
4.000	0.114	0.394	1.809
4.125	0.141	0.381	1.833
4.250	0.154	0.360	1.840
4.375	0.151	0.329	1.834
4.500	0.136	0.302	1.834
4.625	0.179	0.236	1.815
4.750	0.227	0.126	1.776

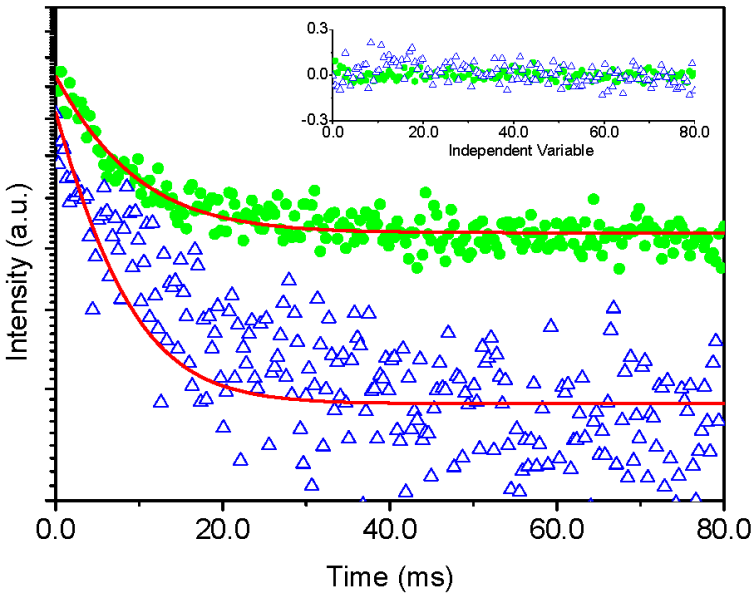

Figure S1. Emission decay curves of 1 excited at 355 nm, monitored at 578 nm and acquired at (green circles) 300 K and at (open triangles) 14 K. The solid lines correspond to the data best fit. The inset shows the best-fit residual plots.

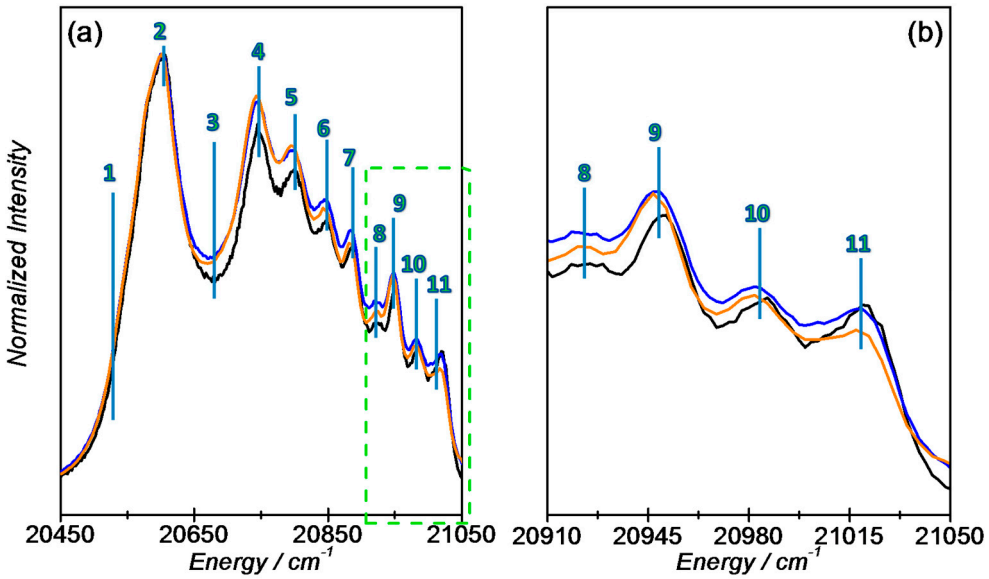

Figure S2. (**a**) Emission spectra in the region of the $^4F_{9/2} \rightarrow {}^6H_{15/2}$ transition acquired at 14 K and excited at 385 nm for 3 distinct ensemble of crystals; (**b**) Magnification of the $^4F_{9/2} \rightarrow {}^6H_{15/2}$ transition high-energy region. From these data three distinct values of ΔE are quantified: (orange line) 32 ± 5 cm^{-1}, (blue line) 34 ± 5 cm^{-1} and (black line), 36 ± 5 cm^{-1}, yielding an average value of 34 ± 5 cm^{-1}.