

## **Sensitive magnetic-field-response magnetization dynamics in a one-dimensional dysprosium coordination polymer**

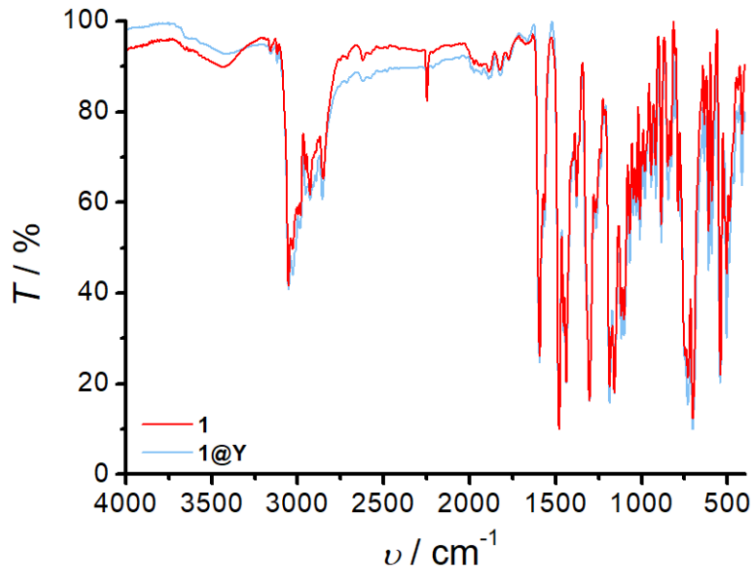
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## 1. Experimental section



**Figure S1.** Infrared spectra for **1** and **1@Y**.

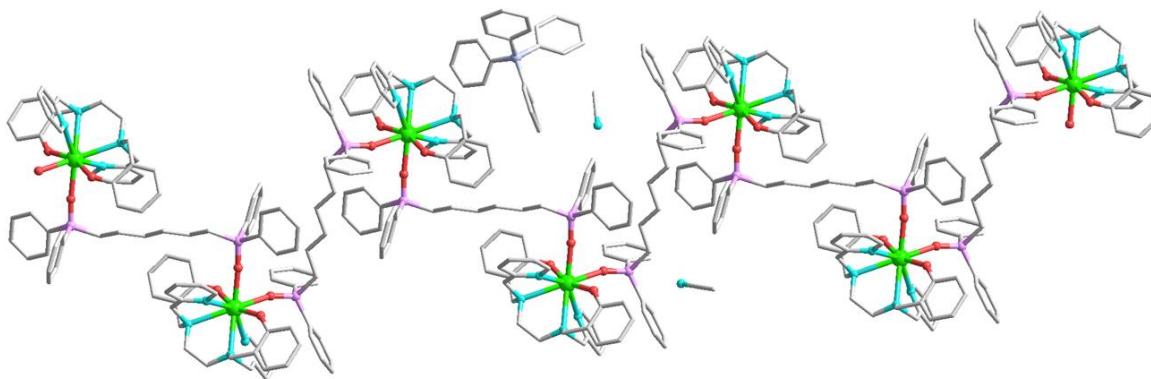
### Computational Details.

All *ab initio* calculations were carried out with OpenMOLCAS version 18.09<sup>1</sup> and are of the CASSCF/RASSI type. The Cholesky decomposition threshold was set to  $1 \times 10^{-8}$  to save disk space. A fragment of polymer, in which the hexylene groups being replaced with propyl groups, was included, and the coordinates of atoms were extracted from the experimentally determined crystal structure. ANO-RCC-VTZP basis set approximations have been employed for Dy, P, O and N atoms, ANO-RCC-VTZ for C and H atoms.<sup>2-4</sup> Active space of the CASSCF method included nine electrons in seven 4f orbitals of Dy(III). 21 sextets were optimized in state-averaged calculations, and then 21 sextets were mixed by spin-orbit coupling using RASSI approach.<sup>5</sup> The *g*-tensors, energies, main magnetic axis as well as the magnetizations were obtained by SINGLE\_ANISO routine.<sup>6</sup>

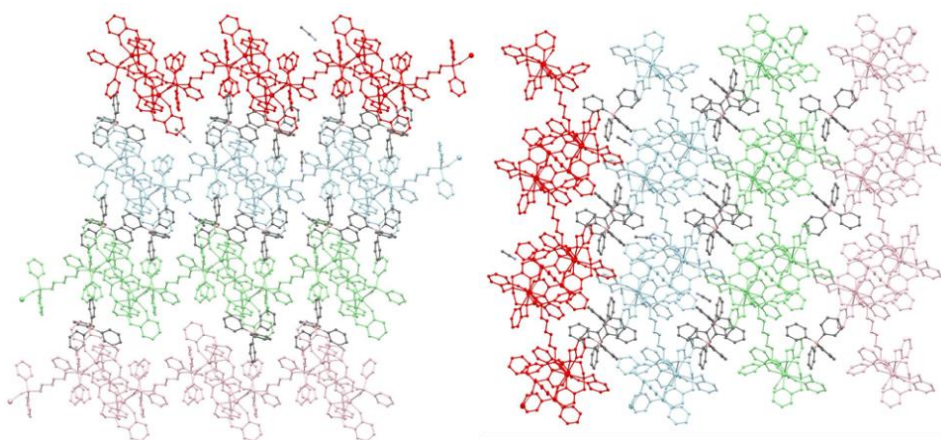
### Magnetic Measurements

Magnetic susceptibility measurements were collected using a Quantum Design MPMS-XL7 SQUID magnetometer and a Quantum Design PPMS, and a Quantum Design MPMS3. Polycrystalline samples were embedded in vaseline to prevent torqueing. All data were corrected for the diamagnetic contribution.

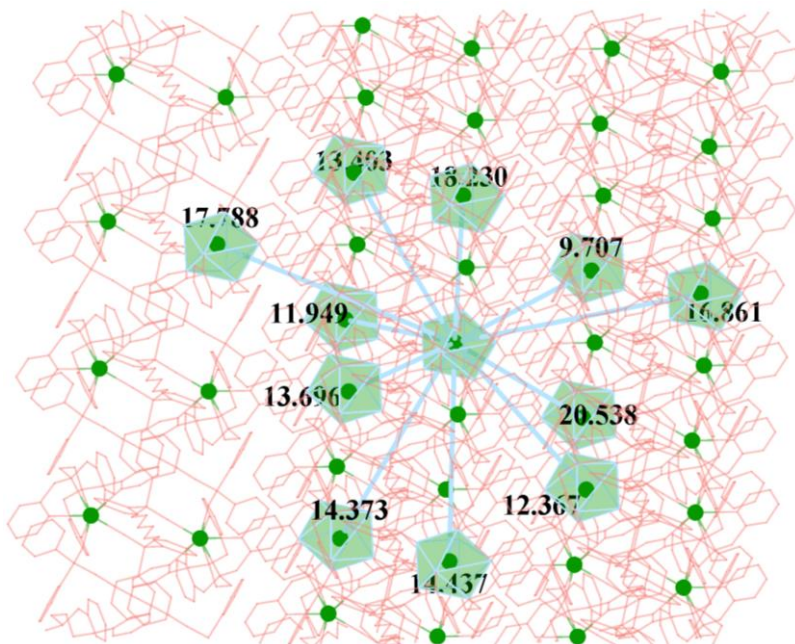
## 2. Crystal Data and Structures



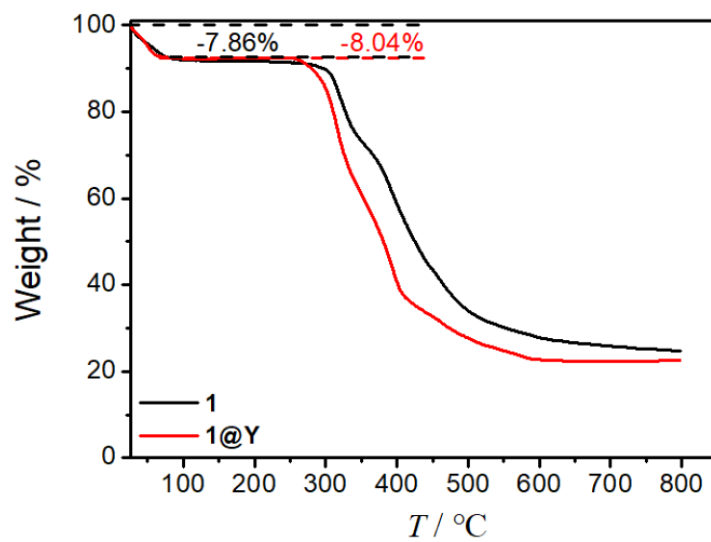
**Figure S2.** 1D crystal structure of **1**. Color Codes: Dy, green; N, blue; P, purplish red; B, purple; O, red; C, gray. Hydrogen atoms are omitted for clarity.



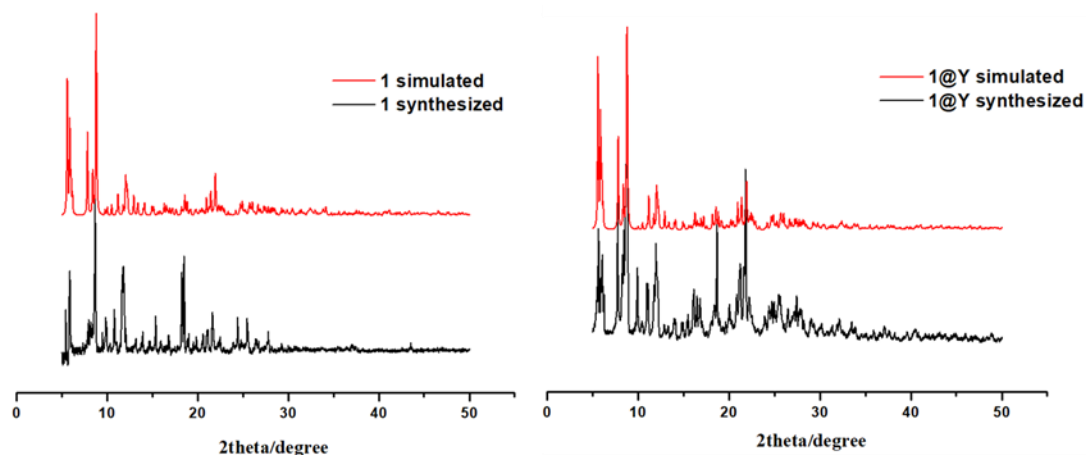
**Figure S3.** Crystal structure of **1** viewed along the *b* and *c* axis. H atoms are omitted for clarity.



**Figure S4.** Intermolecular Dy-Dy distances, where the shortest one is 9.707 Å.



**Figure S5.** Thermogravimetric analysis for **1** and **1@Y** under N<sub>2</sub> atmosphere (10 K min<sup>-1</sup>). The dashed lines correspond to the theoretical weight loss percentage of 2 MeCN and 2 H<sub>2</sub>O.



**Figure S6.** PXRD patterns of **1** (left) and **1@Y** (right) compared with the simulated pattern from the single-crystal structures.

**Table S1.** Continuous Shape Measures calculations (CShM) for **1** and **1@Y**.<sup>7</sup>

| Complex    | OP<br>( <i>D</i> <sub>8h</sub> ) | HPY-8<br>( <i>C</i> <sub>7v</sub> ) | HBPY-8<br>( <i>D</i> <sub>6h</sub> ) | CU-8<br>( <i>O</i> <sub>h</sub> ) | SAPR-8<br>( <i>D</i> <sub>4d</sub> ) | TDD-8<br>( <i>D</i> <sub>3d</sub> ) | JGBF-8<br>( <i>D</i> <sub>3d</sub> ) |
|------------|----------------------------------|-------------------------------------|--------------------------------------|-----------------------------------|--------------------------------------|-------------------------------------|--------------------------------------|
| <b>1</b>   | 32.61912                         | 21.14305                            | 11.98907                             | 8.17713                           | 1.61131                              | 2.56987                             | 11.95869                             |
| <b>1@Y</b> | 32.63058                         | 21.15545                            | 12.05724                             | 8.18014                           | 1.57190                              | 2.56161                             | 12.05322                             |

| Complex    | JETBPY-8<br>( <i>D</i> <sub>3h</sub> ) | JBTPR-8<br>( <i>C</i> <sub>2v</sub> ) | BTPR-8<br>( <i>C</i> <sub>2v</sub> ) | JSD-8<br>( <i>D</i> <sub>2d</sub> ) | TT-8<br>( <i>T</i> <sub>d</sub> ) | ETBPY-8<br>( <i>D</i> <sub>3h</sub> ) |
|------------|--|---------------------------------------|--------------------------------------|-------------------------------------|-----------------------------------|---------------------------------------|
| <b>1</b>   | 27.56682                               | 2.90835                               | 2.63793                              | 4.85210                             | 8.98807                           | 23.04509                              |
| <b>1@Y</b> | 27.68220                               | 2.89480                               | 2.61828                              | 4.84097                             | 8.98859                           | 23.16292                              |

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 J26, JETBPY-8 = Johnson elongated triangular bipyramid J14, JBTPR-8 = Biaugmented trigonal prism J50, BTPR-8 = Biaugmented trigonal prism, JSD-8 = Snub diphenoid J84, TT-8 = Triakis tetrahedron, ETBPY-8 = Elongated trigonal bipyramid

**Table S2.** Crystal data and structure refinement parameters for **1** and **1@Y**

|                   | <b>1</b>  | <b>1@Y</b>   |
|-------------------|---|--|
| Empirical formula | C <sub>86</sub> H <sub>90</sub> BDyN <sub>6</sub> O <sub>6</sub> P <sub>2</sub> | C <sub>86</sub> H <sub>90</sub> BN <sub>6</sub> O <sub>6</sub> P <sub>2</sub> Y <sub>0.95</sub> Dy <sub>0.05</sub> |
| Formula weight    | 1538.88   | 1469.02  |
| Temperature/K     | 120(2)  | 150(2)   |
| Crystal system    | triclinic   | triclinic  |
| Space group       | <i>P</i> -1   | <i>P</i> -1  |
| <i>a</i> /Å       | 14.4368(9)  | 14.4603(10)  |
| <i>b</i> /Å       | 16.8612(11)   | 16.8841(13)  |
| <i>c</i> /Å       | 17.7877(13)   | 17.8153(13)  |

|  |   |   |
|--|---|---|
| $\alpha/^\circ$                                    | 116.577(2)  | 116.529(2)  |
| $\beta/^\circ$                                     | 95.674(2)   | 95.822(2)   |
| $\gamma/^\circ$                                    | 90.602(2)   | 90.434(2)   |
| Volume/ $\text{\AA}^3$                             | 3846.1(5)   | 3864.7(5)   |
| $Z$  | 2   | 2   |
| $\rho_{\text{calc}}/\text{g cm}^{-3}$              | 1.329   | 1.231   |
| $\mu/\text{mm}^{-1}$                               | 1.070   | 0.860   |
| $F(000)$   | 1594  | 1503  |
| Radiation/ $\text{\AA}$                            | Mo- $K\alpha$ ( $\lambda = 0.71073$ )                             | Mo- $K\alpha$ ( $\lambda = 0.71073$ )                             |
| Reflections collected                              | 14686   | 43447   |
| Independent reflections                            | 17620 [ $R_{\text{int}} = 0.0754$ , $R_{\text{sigma}} = 0.0565$ ] | 14290 [ $R_{\text{int}} = 0.0839$ , $R_{\text{sigma}} = 0.0918$ ] |
| Goodness-of-fit on $F^2$                           | 1.037   | 1.005   |
| Final $R$ indexes [ $I \geq 2\sigma(I)$ ]          | $R_1 = 0.0324$ , $wR_2 = 0.0649$                                  | $R_1 = 0.0490$ , $wR_2 = 0.0985$                                  |
| Final $R$ indexes [all data]                       | $R_1 = 0.0478$ , $wR_2 = 0.0691$                                  | $R_1 = 0.0985$ , $wR_2 = 0.1156$                                  |
| Largest diff. peak/hole/ $\text{e}\text{\AA}^{-3}$ | 0.62/−0.80  | 0.39/−0.75  |
| CCDC no.   | 1975686   | 2031584   |

$$^a R_1 = \frac{\sum |F_o| - |F_c|}{\sum |F_o|};$$

$$^b wR_2 = \left\{ \frac{\sum w(F_o^2 - F_c^2)^2}{\sum [w(F_o^2)^2]} \right\}^{1/2}.$$

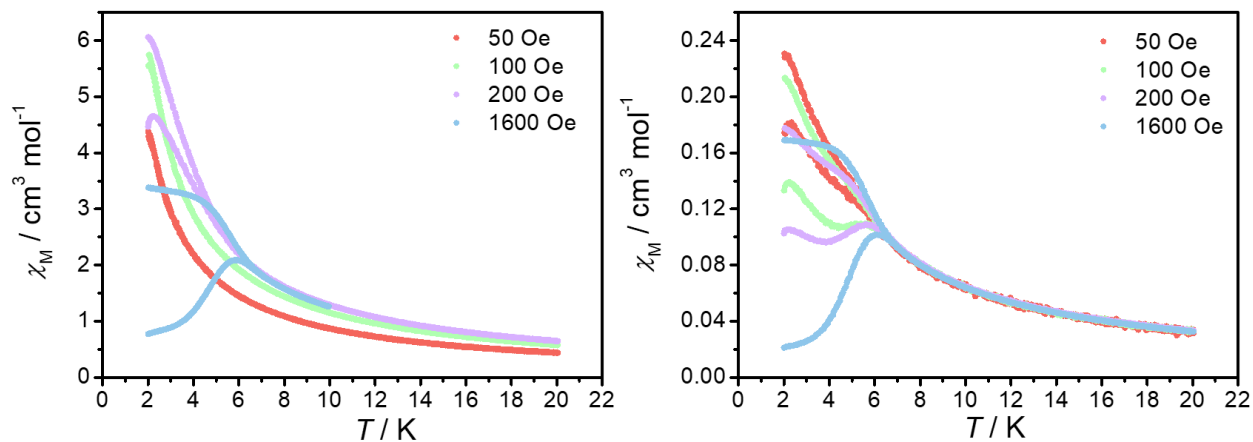
**Table S3.** Selected bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for **1** and **1@Y**

| Bond lengths | <b>1</b>   | <b>1@Y</b> | Bond angles | <b>1</b>  | <b>1@Y</b> |
|--------------|------------|------------|-------------|-----------|------------|
| Dy-N1        | 2.5841(19) | 2.577(3)   | N1-Dy-N2    | 62.46(6)  | 62.40(8)   |
| Dy-N2        | 2.674(2)   | 2.672(3)   | N1-Dy-N3    | 83.16(6)  | 82.96(8)   |
| Dy-N3        | 2.6725(19) | 2.669(3)   | N3-Dy-N2    | 68.04(6)  | 67.88(8)   |
| Dy-N4        | 2.5784(19) | 2.565(3)   | N4-Dy-N1    | 140.45(6) | 140.09(8)  |
| Dy-O1        | 2.2116(17) | 2.213(2)   | N4-Dy-N2    | 86.57(6)  | 86.15(8)   |
| Dy-O2        | 2.2244(17) | 2.221(2)   | N4-Dy-N3    | 61.64(6)  | 61.63(8)   |
| Dy-O3        | 2.3567(16) | 2.343(2)   | O1-Dy-N1    | 80.33(6)  | 80.52(8)   |
| Dy-O4        | 2.3127(15) | 2.298(2)   | O1-Dy-N2    | 126.58(6) | 126.52(8)  |
|              |            |            | O1-Dy-N3    | 70.85(6)  | 70.68(8)   |
|              |            |            | O1-Dy-N4    | 102.48(6) | 102.49(8)  |
|              |            |            | O1-Dy-O2    | 159.92(6) | 160.10(8)  |
|              |            |            | O1-Dy-O3    | 81.99(6)  | 81.81(7)   |
|              |            |            | O1-Dy-O4    | 83.94(6)  | 84.20(7)   |
|              |            |            | O2-Dy-N1    | 107.91(6) | 107.83(8)  |
|              |            |            | O2-Dy-N2    | 72.60(6)  | 72.55(8)   |
|              |            |            | O2-Dy-N3    | 127.46(6) | 127.41(8)  |

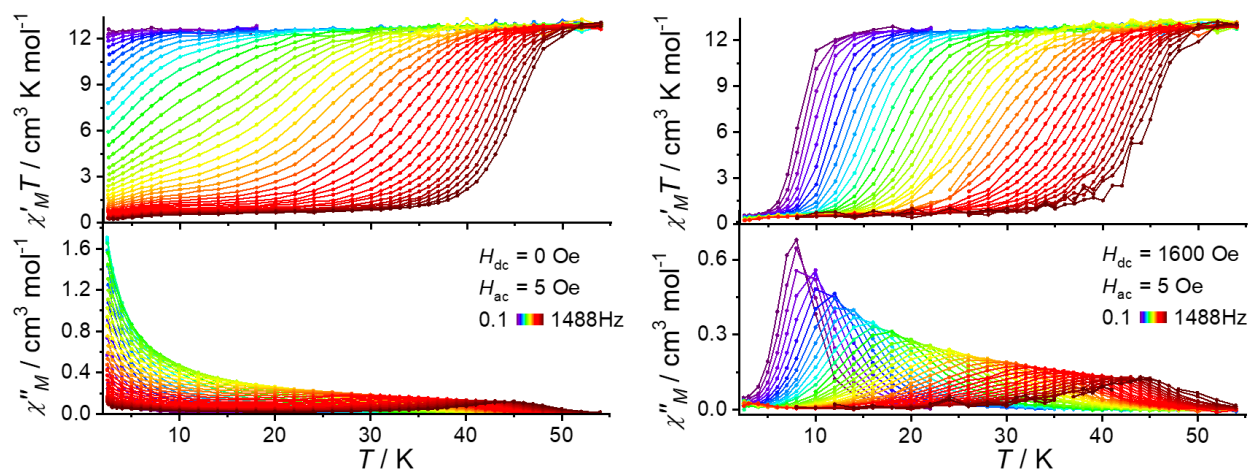
|          |           |           |
|----------|-----------|-----------|
| O2-Dy-N4 | 82.99(6)  | 82.86(8)  |
| O2-Dy-O3 | 81.43(6)  | 81.72(7)  |
| O2-Dy-O4 | 81.83(6)  | 81.86(7)  |
| O3-Dy-N1 | 145.98(6) | 146.30(7) |
| O3-Dy-N2 | 148.13(6) | 148.11(7) |
| O3-Dy-N3 | 117.73(6) | 117.49(8) |
| O3-Dy-N4 | 71.95(6)  | 71.98(8)  |
| O4-Dy-N1 | 70.51(6)  | 70.49(8)  |
| O4-Dy-N2 | 114.33(6) | 114.29(8) |
| O4-Dy-N3 | 146.28(6) | 146.15(8) |
| O4-Dy-N4 | 148.80(6) | 149.13(8) |
| O4-Dy-O3 | 78.92(5)  | 79.37(7)  |

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### 3. Magnetic Characterization

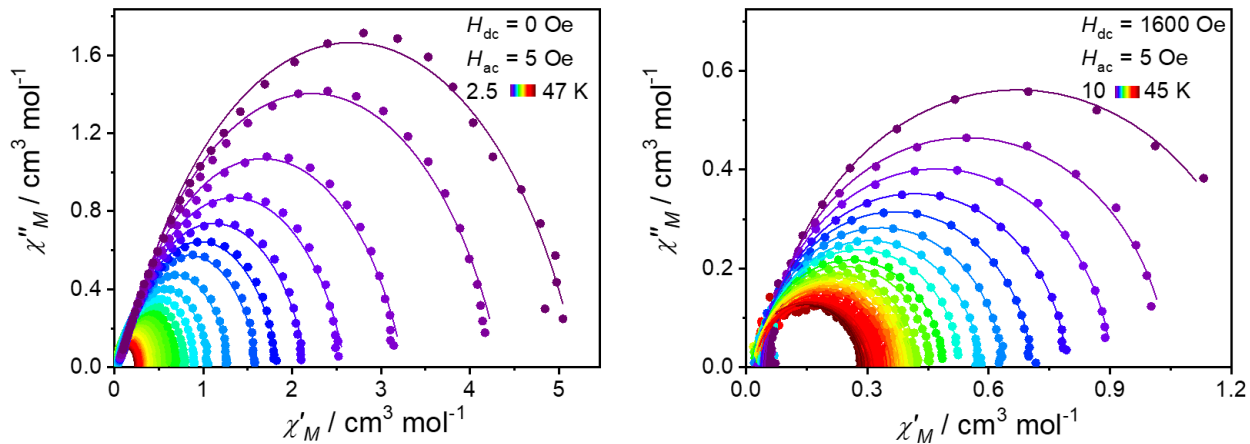


**Figure S7.** Zero-field-cooled/field-cooled (ZFC-FC) magnetic susceptibilities (warm mode,  $2 \text{ K min}^{-1}$ ) for **1** (left) and **1@Y** (right).

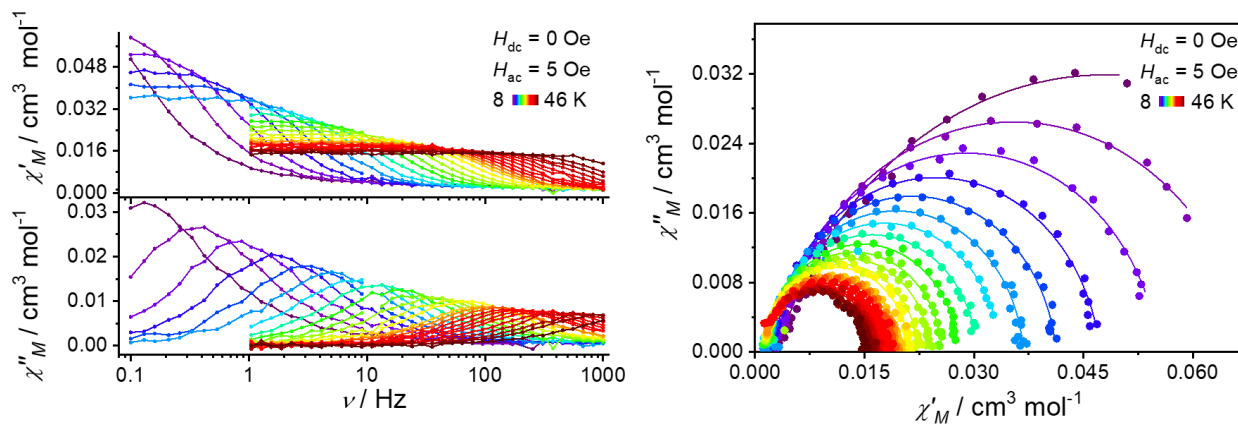


**Figure S8.** Temperature dependence of the in-phase ( $\chi'_M T$ ) and out-of-phase ( $\chi''_M$ ) components of the ac magnetic susceptibility for **1** under 0 (left) and 1600 Oe (right) applied dc field with the ac frequency of 0.1-1488 Hz.

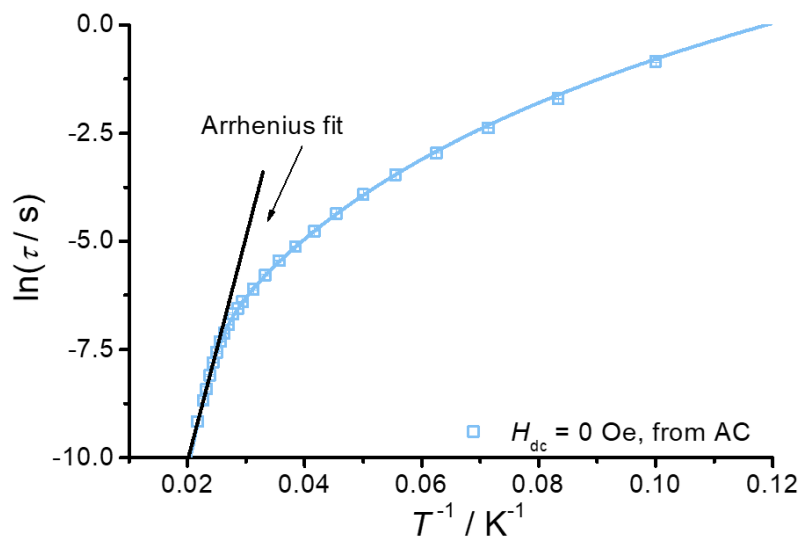




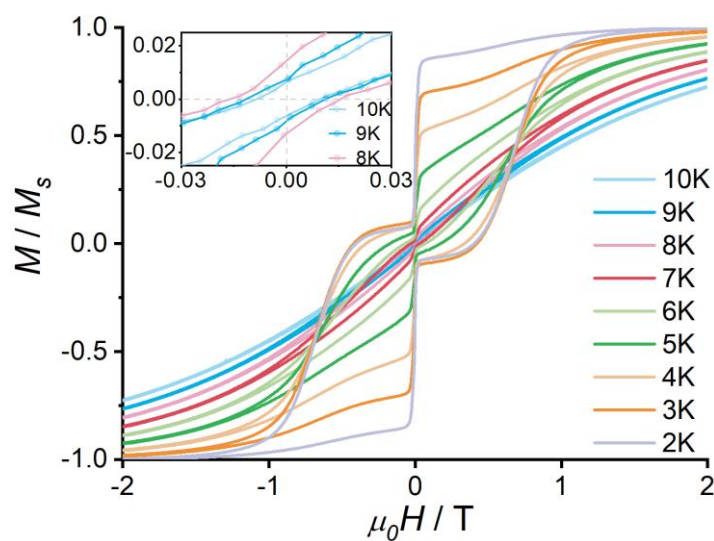
**Figure S9.** Cole-Cole plots for the determination of the temperature dependence of  $\tau$  for pure **1** under zero (*left*) and 1600 Oe (*right*) dc applied field. Solid lines are the results of best fits to the generalized Debye model as described in the main text.



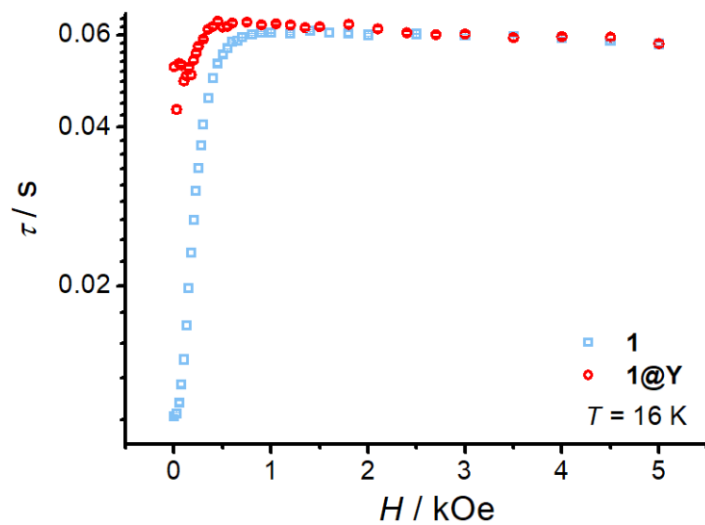
**Figure S10.** Frequency-dependence of the in-phase ( $\chi'_M T$ ) product and out-of-phase ( $\chi''_M$ ) under zero dc field for **1@Y** with the ac frequency of 0.1-999 Hz. The solid lines are guides for the eyes (*left*). Cole-Cole plots of **1@Y** at 8-46 K under zero dc field ( $\alpha = 0-0.214$ ), and solid lines are best fits for the generalized Debye model (*right*).



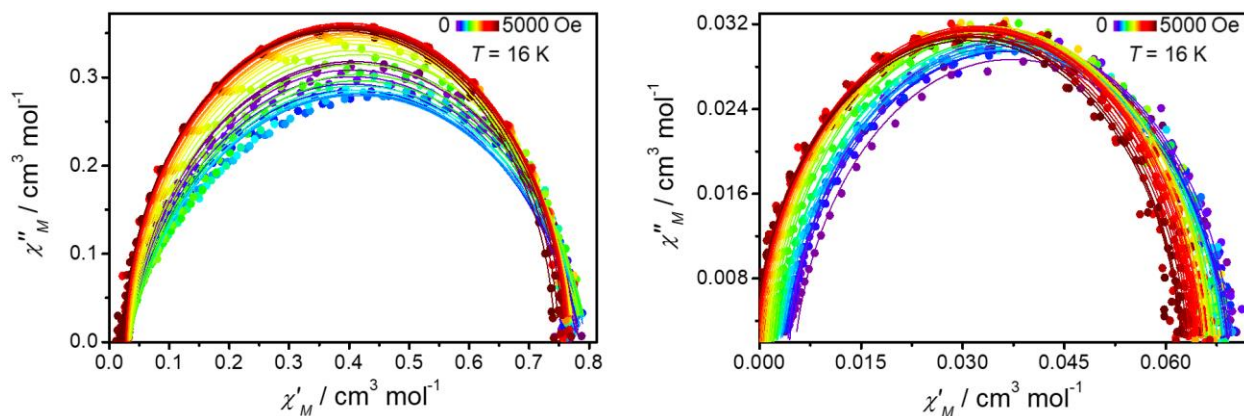
**Figure S11.** Temperature dependence of the relaxation time  $\tau$  under zero dc field for **1@Y**. The solid lines are best fits to the Arrhenius law, and the dashed lines are best fits to the multiple relaxation equation.



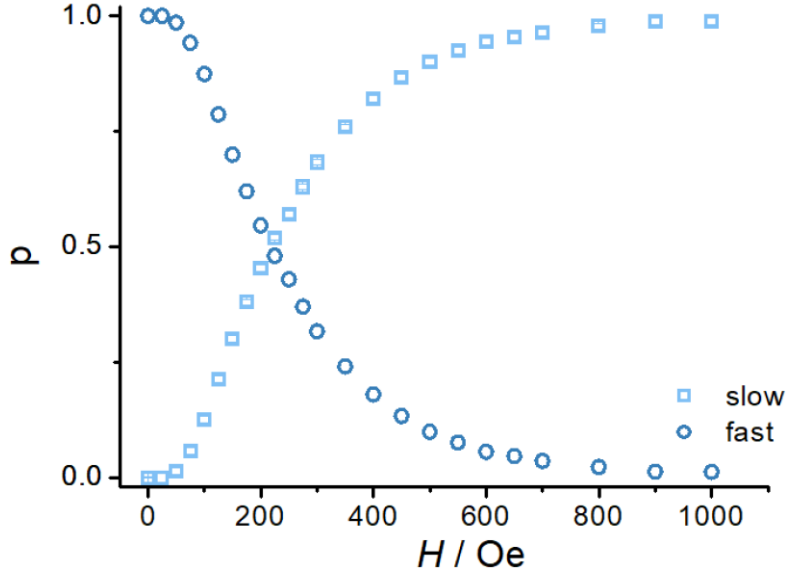
**Figure S12.** Normalized magnetic hysteresis loops for **1@Y**. The data were continuously collected at intervals of 1 s with the field ramping speed of 200 Oe/s at various temperatures. The expanded views (inset) reveal clear magnetic hysteresis to 9 K. For all temperatures below, the loops are open at zero field.



**Figure S13.** Field dependence of the relaxation time for **1** and **1@Y** extracted from the single-relaxation-time model.



**Figure S14.** Cole-Cole plots of **1** (*left*) and **1@Y** (*right*) at 16 K under 0-5000 Oe dc field, and solid lines are best fits for the generalized Debye model.



**Figure S15.** Field dependence of the relaxation time for **1** extracted from the double-relaxation-time model<sup>8</sup>.  $p$  is the proportion of two relaxation times: one is fast relaxation (deep blue); another is slow one (light), with  $\tau_1 = 0.0595(2)$  s,  $\tau_2 = 0.01179(7)$  s, respectively.

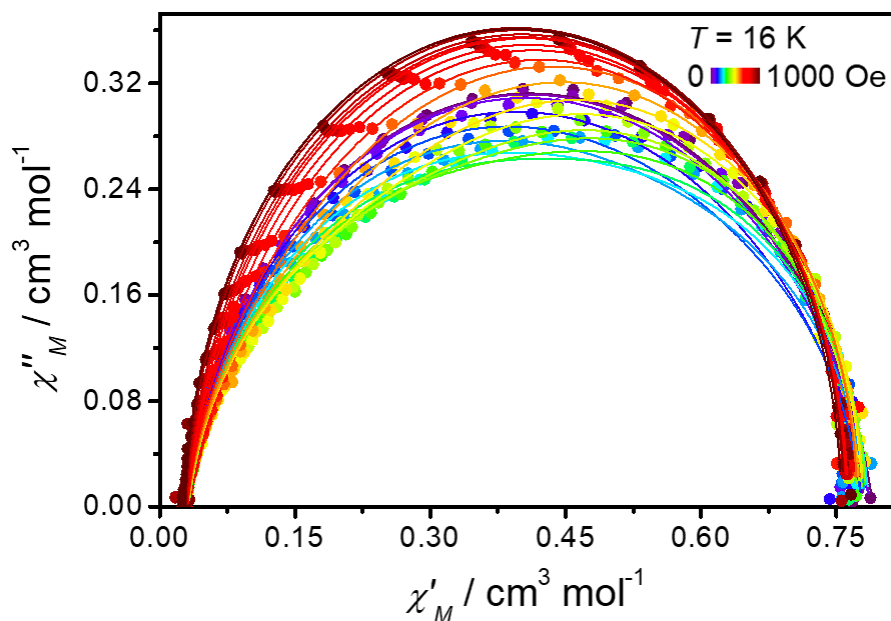
The formula of double-relaxation-time model is shown as follows:

$$\chi(\omega) = \chi_s + p \frac{\chi_T - \chi_s}{1 + (i\omega\tau_1)^{1-\alpha}} + (1-p) \frac{\chi_T - \chi_s}{1 + (i\omega\tau_2)^{1-\alpha}} \quad \text{Eqn(S1)}$$

$$\begin{aligned} \chi'(\omega) = & \chi_s + p (\chi_T - \chi_s) \frac{1 + (\omega\tau_1)^{1-\alpha_1} \sin(\pi\alpha_1/2)}{1 + 2(\omega\tau_1)^{1-\alpha_1} \sin(\pi\alpha_1/2) + (\omega\tau_1)^{2-2\alpha_1}} \\ & + (1-p)(\chi_T - \chi_s) \frac{1 + (\omega\tau_2)^{1-\alpha_2} \sin(\pi\alpha_2/2)}{1 + 2(\omega\tau_2)^{1-\alpha_2} \sin(\pi\alpha_2/2) + (\omega\tau_2)^{2-2\alpha_2}} \end{aligned}$$

$$\begin{aligned} \chi''(\omega) = & p (\chi_T - \chi_s) \frac{(\omega\tau_1)^{1-\alpha_1} \cos(\pi\alpha_1/2)}{1 + 2(\omega\tau_1)^{1-\alpha_1} \sin(\pi\alpha_1/2) + (\omega\tau_1)^{2-2\alpha_1}} \\ & + (1-p)(\chi_T - \chi_s) \frac{(\omega\tau_2)^{1-\alpha_2} \cos(\pi\alpha_2/2)}{1 + 2(\omega\tau_2)^{1-\alpha_2} \sin(\pi\alpha_2/2) + (\omega\tau_2)^{2-2\alpha_2}} \end{aligned}$$

$\chi_T$  and  $\chi_s$  are the isothermal and adiabatic limit of the susceptibility, respectively. The wider the distribution in relaxation times the larger is  $\alpha$ , and  $\alpha_1 = 0.000(3)$ ,  $\alpha_2 = 0.125(2)$ .



**Figure S16.** Cole-Cole plots of **1** at 16 K under 0-1000 Oe dc field, and the solid lines are best fits for the double-relaxation-time model.

**Table S4.** Selected 1D structures and their effective energy barrier.

| Compound   | $U_{\text{eff}}/k_B$ [K] | References       |
|--|--------------------------|------------------|
| [Mn <sub>2</sub> Ni <sub>3</sub> Cl <sub>2</sub> L <sub>4</sub> (LH) <sub>2</sub> (H <sub>2</sub> O) <sub>2</sub> ]  | 27                       | 9                |
| {KDy(C <sub>2</sub> O <sub>4</sub> ) <sub>2</sub> (H <sub>2</sub> O) <sub>4</sub> } <sub>n</sub>   | 418                      | 10               |
| [Dy(ppmc) <sub>2</sub> ·4H <sub>2</sub> O]·ppmc·H <sub>2</sub> O   | 74                       | 11               |
| [Dy(L)(H <sub>2</sub> O) <sub>4</sub> ]Cl <sub>2</sub> ·2H <sub>2</sub> O  | 227                      | 12               |
| {[Mn <sup>II</sup> (dapsc)][Mn <sup>III</sup> (CN) <sub>6</sub> ][K(H <sub>2</sub> O) <sub>2.75</sub> -(MeOH) <sub>0.5</sub> ]} <sub>n</sub> ·0.5n(H <sub>2</sub> O) | 40                       | 13               |
| [Dy(μ-H <sub>2</sub> O)(phen)(μ-OH)(nb) <sub>2</sub> ] <sub>n</sub>  | 88.7                     | 14               |
| [Dy(L) <sub>2</sub> (phen)(μ <sub>2</sub> -OH)(μ <sub>2</sub> -H <sub>2</sub> O)] <sub>n</sub>   | 567                      | 15               |
| {[DyZn <sub>2</sub> (L <sup>a</sup> ) <sub>2</sub> (POC)](OH)(ClO <sub>4</sub> )}·H <sub>2</sub> O·MeOH  | 235                      | 16               |
| [TbCu <sub>2</sub> (hfac) <sub>7</sub> (bisNITPhPy)] <sub>n</sub>  | 26                       | 17               |
| [Dy <sub>2</sub> (μ <sub>3</sub> -cpdc)(μ <sub>2</sub> -bc)(H <sub>2</sub> O)] <sub>n</sub>  | 55                       | 18               |
| [Yb <sub>2</sub> (DAPBH) <sub>2</sub> (DPP) <sub>3</sub> (CH <sub>3</sub> OH)](NO <sub>3</sub> )(ClO <sub>4</sub> ) <sub>2</sub> ·3CH <sub>3</sub> OH                | 7                        | 19               |
| {[Dy(DAPMBH)(N <sub>3</sub> )C <sub>2</sub> H <sub>5</sub> OH]C <sub>2</sub> H <sub>5</sub> OH] <sub>n</sub>   | 47                       | 20               |
| Co(hfac) <sub>2</sub> (EtONapNIT)  | 368                      | 21               |
| <b>[Dy(bbpen)(dppHO<sub>2</sub>)](BPh<sub>4</sub>)·2MeCN·2H<sub>2</sub>O</b>   | <b>691</b>               | <b>This work</b> |

## 4. Photoluminescence Spectra

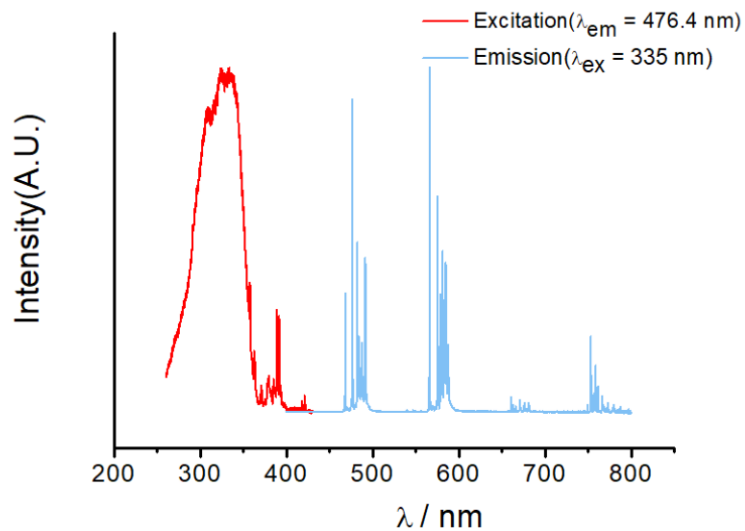


Figure S17. Photoluminescence spectra for **1** at 5 K.

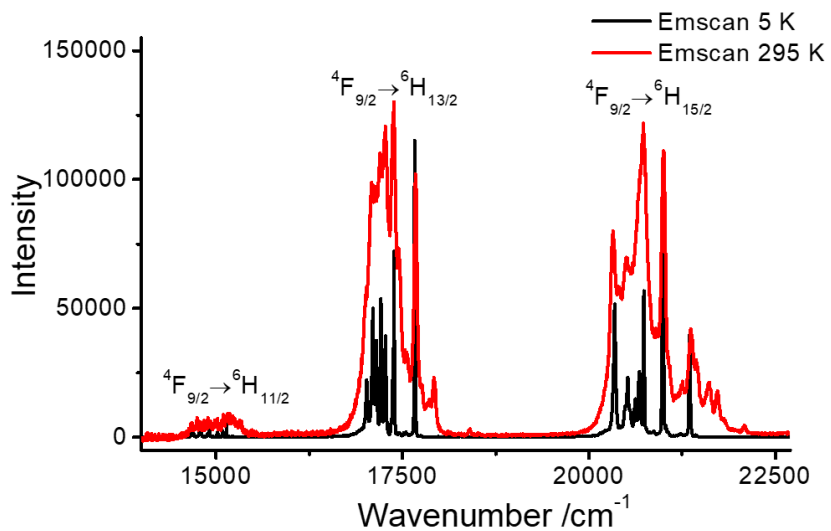
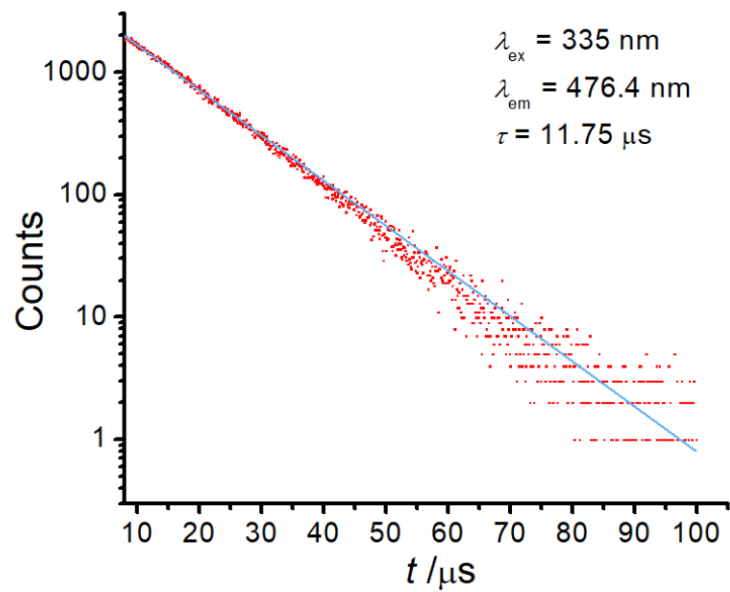
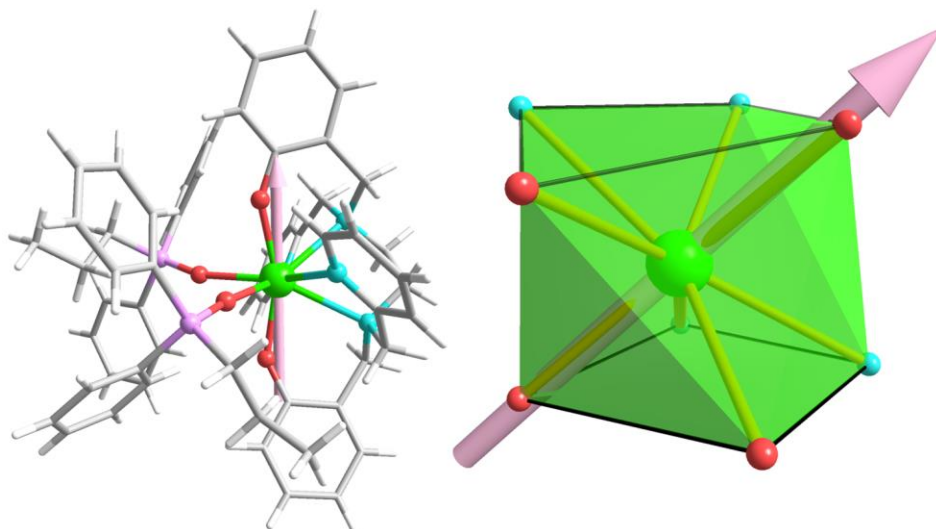


Figure S18. The emission spectra were measured at 295 K ( $\lambda_{ex} = 350$  nm) and 5 K ( $\lambda_{ex} = 335$  nm) for **1**.

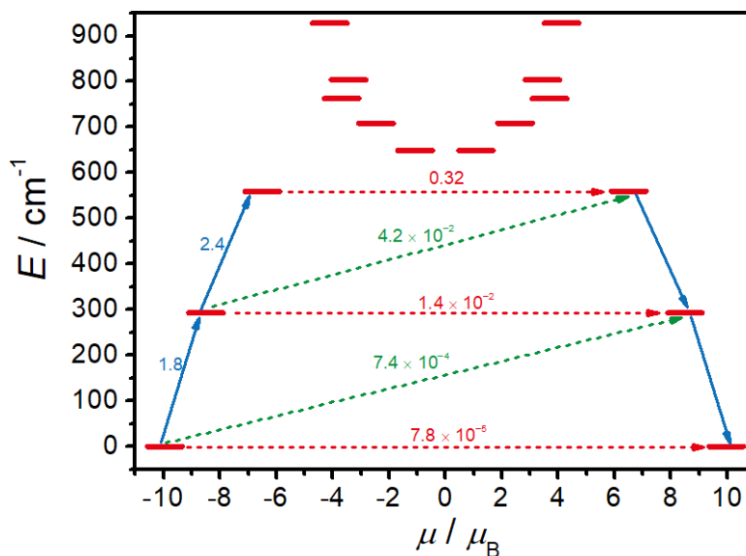


**Figure S19.** Lifetime measurements were collected at 5 K with mean lifetime  $\tau = 11.75(3) \mu\text{s}$  (by first order exponential fits) for **1**.

## 5. *Ab Initio* Calculations



**Figure S20.** The fragment of single-crystal structure of **1** used for the *ab initio* calculations (*left*). The main magnetic axis of the ground Kramers doublet (pink arrow) is roughly along the pair of phenols' oxygen atoms and the central Dy displays distorted square antiprism geometry with the orientation of the main magnetic axis (*right*).



**Figure S21.** Magnetization blocking barriers for complex **1**. The lowest 16 spin-orbit states are arranged according to the magnitude of their magnetic moments on the horizontal axis. The numbers next to arrows connecting two states display the average transition magnetic moment matrix element between the respective states.



**Table S5.** Energies ( $\text{cm}^{-1}$ ),  $g$ -tensors ( $g_x, g_y, g_z$ ) and angles ( $^\circ$ ) between the main magnetic axes of the selected Kramers doublet and the ground Kramers doublet for the local Dy(III) site in **1**.

| <b>KD</b> | <b><i>E</i></b> | <b><i>g</i></b> | <b>angle</b> |
|-----------|-----------------|-----------------|--------------|
| <b>1</b>  | 0               | 0.0002          | 0            |
|           |                 | 0.0003          |              |
|           |                 | 19.921          |              |
| <b>2</b>  | 292.477         | 0.0394          | 2.363        |
|           |                 | 0.0424          |              |
|           |                 | 17.008          |              |
| <b>3</b>  | 559.088         | 0.6459          | 5.769        |
|           |                 | 1.2224          |              |
|           |                 | 13.060          |              |
| <b>4</b>  | 648.725         | 1.1230          | 83.502       |
|           |                 | 3.4630          |              |
|           |                 | 15.077          |              |
| <b>5</b>  | 708.554         | 2.1636          | 69.696       |
|           |                 | 4.0088          |              |
|           |                 | 11.019          |              |
| <b>6</b>  | 762.568         | 1.2792          | 45.052       |
|           |                 | 3.5893          |              |
|           |                 | 9.8967          |              |
| <b>7</b>  | 803.599         | 1.0015          | 62.853       |
|           |                 | 3.3770          |              |
|           |                 | 14.791          |              |
| <b>8</b>  | 928.072         | 0.0956          | 64.946       |
|           |                 | 0.2017          |              |
|           |                 | 19.400          |              |

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