Electronic Supplementary Material (ESI) for CrystEngComm.
This journal is © The Royal Society of Chemistry 2021

Electronic Supplementary Information (ESI) for *CrystEngComm*

# Regulating the Distortion Degree of the Square Antiprism Coordination Geometry in the Dy-Na Single Ion Magnets

Hui-Sheng Wang,[*a] Ke Zhang,[a] Jia Wang,[b] Zhaobo Hu,[b] You Song,[*b] Zaichao Zhang,[c] and Zhi-Quan Pan[a]

[a]School of Chemistry and Environmental Engineering, Key Laboratory of Green Chemical Process of Ministry of Education, Key Laboratory of Novel Reactor and Green Chemical Technology of Hubei Province, Wuhan Institute of Technology, Wuhan 430205, P. R. China.

[b]State Key Laboratory of Coordinate Chemistry, Nanjing National Laboratory of Microstructures, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, P. R. China.

[c]Jiangsu Key Laboratory for the Chemistry of Low-dimensional Materials, School of Chemistry and Chemical Engineering, Huaiyin Normal University, P. R. China.

[*]Email: wangch198201@163.com (H.-S. W.).

[*]Email: yousong@nju.edu.cn (Y. S.)

# Contents

**Table S1**. Crystal data and structure refinement parameters for complexes **1-2**.

| Compounds | **1** | **2** |
|---|---|---|
| Formula[a] | $C_{46}H_{44}DyN_4NaO_{10}$ | $C_{46}H_{44}DyN_5Na_2O_{13}$ |
| Formula weight | 998.34 | 1083.34 |
| Crystal color | yellow | yellow |
| Crystal size (mm) | 0.51×0.32×0.06 | 0.18×0.17×0.14 |
| Crystal system | monoclinic | monoclinic |
| Space group | $P\ 2_1/c$ | $P\ 2_1/c$ |
| $a$ (Å) | 22.3221(6) | 10.9971(4) |
| $b$ (Å) | 11.7740(3) | 29.7015(10) |
| $c$ (Å)) | 16.2459(4) | 14.6760(4) |
| $\alpha$ (°) | 90 | 90 |
| $\beta$ (°) | 90.1500(10) | 111.4410(10) |
| $\gamma$ (°) | 90 | 90 |
| Unit cell volume (Å3) | 4269.74(19) | 4461.9(3) |
| $T$ (K) | 173(2) | 173(2) |
| $Z$ | 4 | 4 |
| Radiation type | Mo/$K\alpha$ | Mo/$K\alpha$ |
| $\mu$ ($mm^{-1}$) | 1.825 | 1.767 |
| $D$c/g ($cm^{-3}$) | 1.553 | 1.613 |
| $\theta$ range | 2.74-25.34 | 2.74- 25.33 |
| Index ranges | $-26 \le h \le 26$ | $-13 \le h \le 13$ |
| | $-14 \le k \le 14$ | $-35 \le k \le 35$ |
| | $-15 \le l \le 15$ | $-17 \le l \le 17$ |
| $F$(000) | 2020 | 2188 |
| Reflections collected | 35053 | 25671 |
| Unique reflections [Rint] | 7474 | 7813 |
| Reflections with $I > 2\sigma(I)$ | 4608 | 6085 |
| Final $R$ indices ($I > 2\sigma(I)$[b,c] | $R_1 = 0.0471$,w$R_2 = 0.0881$ | $R_1 = 0.0349$,w$R_2 = 0.0712$ |
| Final $R$ indices (all data) | $R_1 = 0.0964$,w$R_2 = 0.1019$ | $R_1 = 0.0553$,w$R_2 = 0.0765$ |
| $S$ (all data) | 1.085 | 1.025 |

[a] The formula and the formula weights include the MeOH solvent molecules which were free.

[b] $R_1 = \Sigma\ (||F_o| - |F_c||)/\Sigma|F_o|$.

[c] $wR_2 = [\ \Sigma\ [w\ (F_o^2 - F_c^2)^2]/\ \Sigma\ [w\ (F_o^2)^2]]^{0.5}$, $w = 1/[\sigma^2(F_o^2) + [(ap)^2 + bp]$, where $p = [\max(F_o^2, 0) + 2F_c^2]/3$.

**Table S2**. Selected bond lengths (Å) and angles (°) for **1**.

| Selected bond lengths for **1** | | | | | |
|---|---|---|---|---|---|
| Dy1-O5 | 2.269(4) | Dy1-N4 | 2.531(5) | Na1-O6 | 2.414(5) |
| Dy1-O6 | 2.276(4) | Dy1-N2 | 2.531(5) | Na1-O4 | 2.514(6) |
| Dy1-O1 | 2.275(4) | Dy1-N1 | 2.550(5) | Na1-O2 | 2.528(5) |
| Dy1-O2 | 2.285(4) | Na1-O5 | 2.343(5) | Na1-O7 | 2.679(5) |
| Dy1-N3 | 2.496(5) | Na1-O10 | 2.373(6) | Na1-O8 | 2.720(6) |
| Selected bond angles for **1** | | | | | |
| O5-Dy1-O6 | 74.34(15) | O5-Dy1-N3 | 72.07(16) | O5-Na1-O4 | 117.47(19) |
| O6-Dy1-O1 | 156.31(14) | O1-Dy1-N3 | 79.19(17) | O5-Na1-O2 | 72.77(16) |
| O5-Dy1-O2 | 78.87(16) | O6-Dy1-N4 | 69.79(16) | O6-Na1-O2 | 69.89(16) |
| O1-Dy1-O2 | 88.56(17) | N3-Dy1-N1 | 82.77(17) | O5-Na1-O7 | 62.04(15) |
| O5-Dy1-N3 | 72.07(16) | N4-Dy1-N1 | 71.86(17) | O10-Na1-O7 | 81.40(18) |
| O1-Dy1-N3 | 79.19(17) | N2-Dy1-N1 | 63.08(17) | O6-Na1-O7 | 127.07(19) |
| O1-Dy1-N4 | 129.91(17) | O5-Na1-O10 | 132.3(2) | O4-Na1-O7 | 98.30(19) |
| O5-Dy1-O2 | 78.87(16) | O5-Na1-O6 | 70.50(16) | O10-Na1-O6 | 118.5(2) |
| O1-Dy1-O2 | 88.56(17) | | | | |

**Table S3**. Selected bond lengths (Å) and angles (°) for **2**.

| Selected bond lengths for **2** | | | | | |
|---|---|---|---|---|---|
| Dy1-O1 | 2.260(3) | N5-O10 | 1.246(5) | Na1-O4 | 2.844(4) |
| Dy1-O2 | 2.272(3) | N5-Na1 | 2.850(4) | Na2-O6 | 2.436(3) |
| Dy1-O6 | 2.277(3) | N5-Na2 | 2.976(4) | Na2-O5 | 2.456(3) |
| Dy1-O5 | 2.286(3) | Na1-O2 | 2.393(3) | Na2-O9 | 2.483(4) |
| Dy1-N1 | 2.495(4) | Na1-O1 | 2.447(3) | Na2-O2 | 2.635(4) |
| Dy1-N3 | 2.497(3) | Na1-O9 | 2.484(4) | Na2-O11 | 2.681(5) |
| Dy1-N2 | 2.505(4) | Na1-O10 | 2.497(4) | Na2-O8 | 2.712(3) |
| Dy1-N4 | 2.519(3) | Na1-O7 | 2.607(4) | Na2-O4 | 2.721(4) |
| N5-O11 | 1.229(5) | Na1-O5 | 2.757(3) | Na2-N5 | 2.976(4) |
| N5-O9 | 1.241(5) | Na1-O3 | 2.772(4) | | |
| Selected bond angles for **1** | | | | | |
| O1-Dy1-O2 | 78.08(10) | O2-Na1-O1 | 72.27(10) | O5-Na2-O2 | 67.65(10) |
| O2-Dy1-O6 | 78.62(11) | O9-Na1-O10 | 51.02(11) | O11-Na2-O8 | 114.77(12) |
| O6-Dy1-O5 | 75.79(10) | O7-Na1-O5 | 57.63(9) | O9 Na2 O4 | 96.93(14) |
| O1-Dy1-N1 | 71.90(11) | N3-Dy1-N4 | 64.27(11) | O2 Na1 O4 | 57.69(10) |

**Table S4**. The possible geometries of octa-coordination metal centers and Deviation parameters from each ideal polyhedron for Dy in complex **1**.

| Point group | Geometry | Polyhedron | Dy1 |
|---|---|---|---|
| $D_{8h}$ | OP-8 | Octagon | 31.857 |
| $C_{7v}$ | HPY-8 | Heptagonal pyramid | 20.930 |
| $D_{6h}$ | HBPY-8 | Hexagonal bipyramid | 13.836 |
| $O_h$ | CU-8 | Cube | 9.365 |
| $D_{4d}$ | SAPR-8 | Square antiprism | 1.123 |
| $D_{2d}$ | TDD-8 | Triangular dodecahedron | 2.698 |
| $D_{2d}$ | JGBF-8 | Johnson - Gyrobifastigium (J26) | 13.407 |
| $D_{3h}$ | JETBPY-8 | Johnson - Elongated triangular bipyramid (J14) | 27.132 |
| $C_{2v}$ | JBTP-8 | Johnson - Biaugmented trigonal prism (J50) | 3.193 |
| $C_{2v}$ | BTPR-8 | Biaugmented trigonal prism | 2.423 |
| $D_{2d}$ | JSD-8 | Snub disphenoid (J84) | 5.109 |
| $T_d$ | TT-8 | Triakis tetrahedron | 10.117 |
| $D_{3h}$ | ETBPY-8 | Elongated trigonal bipyramid | 22.532 |

**Table S5**. The possible geometries of octa-coordination metal centers and Deviation parameters from each ideal polyhedron for Dy in complex **2**.

| Point group | Geometry | Polyhedron | Dy1 |
|---|---|---|---|
| $D_{8h}$ | OP-8 | Octagon | 32.546 |
| $C_{7v}$ | HPY-8 | Heptagonal pyramid | 22.438 |
| $D_{6h}$ | HBPY-8 | Hexagonal bipyramid | 15.627 |
| $O_h$ | CU-8 | Cube | 10.293 |
| $D_{4d}$ | SAPR-8 | Square antiprism | 0.955 |
| $D_{2d}$ | TDD-8 | Triangular dodecahedron | 2.181 |
| $D_{2d}$ | JGBF-8 | Johnson - Gyrobifastigium (J26) | 14.520 |
| $D_{3h}$ | JETBPY-8 | Johnson - Elongated triangular bipyramid (J14) | 27.771 |
| $C_{2v}$ | JBTP-8 | Johnson - Biaugmented trigonal prism (J50) | 3.074 |
| $C_{2v}$ | BTPR-8 | Biaugmented trigonal prism | 2.526 |
| $D_{2d}$ | JSD-8 | Snub disphenoid (J84) | 5.006 |
| $T_d$ | TT-8 | Triakis tetrahedron | 11.101 |
| $D_{3h}$ | ETBPY-8 | Elongated trigonal bipyramid | 23.244 |

**Table S6**. The details for parameters involved in SAP geometry for **1** and **2**.

| Skew angle ($\emptyset$) of complex **1** (°) | | Skew angle ($\emptyset$) of complex **2** (°) | |
|---|---|---|---|
| $\emptyset$1 = 52.82(1) | $\emptyset$2 = 43.05(1) | $\emptyset$1 = 45.97(9) | $\emptyset$2 = 44.32(1) |
| $\emptyset$3 = 49.22(2) | $\emptyset$4 = 43.91(2) | $\emptyset$3 = 45.23(1) | $\emptyset$4 = 47.18(9) |
| Mean value of $\emptyset$ = 47.25(2) | | Mean value of $\emptyset$ = 45.68(5) | |
| Parameter $\gamma$ and magic angles $\alpha$ for complex **1** (°) | | Parameter $\gamma$ and magic angles $\alpha$ for complex **2** (°) | |
| $\gamma$(O1-Dy1-N2) = 109.62(2) | $\alpha$(O1-N2) = 54.81(1) | $\gamma$(O1-Dy1-N2) = 107.74(1) | $\alpha$(O1-N2) = 53.87(1) |
| $\gamma$(O2-Dy1-N1) = 119.94(2) | $\alpha$(O2-N1) = 59.97(1) | $\gamma$(O2-Dy1-N1) = 114.95(1) | $\alpha$(O2-N1) = 57.48(1) |
| $\gamma$(O5-Dy1-N4) = 111.69(2) | $\alpha$(O5-N4) = 55.85(1) | $\gamma$(O5-Dy1-N4) = 114.71(1) | $\alpha$(O5-N4) = 57.36(1) |
| $\gamma$(O6-Dy1-N3) = 104.09(2) | $\alpha$(O6-N3) = 52.05(1) | $\gamma$(O6-Dy1-N3) = 105.80(1) | $\alpha$(O6-N3) = 52.91(1) |
| Mean value of $\gamma$ = 111.34 | Mean value of $\alpha$ = 55.67 | Mean value of $\gamma$ = 110.80 | Mean value of $\alpha$ = 55.41 |
| Values of $d_{in}$ for **1** (Å) | | Values of $d_{in}$ for **2** (Å) | |
| $d_{in}$(N1-N2) = 2.66(8) | $d_{in}$(N2-O2) = 2.87(6) | $d_{in}$(N1-N2) = 2.65(5) | $d_{in}$(N2-O2) = 2.85(4) |
| $d_{in}$(O1-O2) = 3.18(6) | $d_{in}$(N1-O1) = 2.82(6) | $d_{in}$(O1-O2) = 2.85(4) | $d_{in}$(N1-O1) = 2.80(4) |
| $d_{in}$(N3-N4) = 2.65(6) | $d_{in}$(N4-O6) = 2.76(7) | $d_{in}$(N3-N4) = 2.67(4) | $d_{in}$(N4-O6) = 2.79(5) |
| $d_{in}$(O5-O6) = 2.74(6) | $d_{in}$(N3-O5) = 2.81(7) | $d_{in}$(O5-O6) = 2.80(3) | $d_{in}$(N3-O5) = 2.87(5) |
| Mean value of $d_{in}$ = 2.81(6) | | Mean value of $d_{in}$ = 2.79(4) | |
| $d_{pp}$(A-B) in **1** (Å) | | $d_{pp}$(A-B) in **2** (Å) | |
| $d_{pp}$(N1-B) = 2.82(5) | $d_{pp}$(N2-B) = 2.88(5) | $d_{pp}$(N3-B) = 2.87(3) | $d_{pp}$(N4-B) = 2.96(3) |
| $d_{pp}$(O1-B) = 2.65(4) | $d_{pp}$(O2-B) = 2.33(5) | $d_{pp}$(O5-B) = 2.28(3) | $d_{pp}$(O6-B) = 2.67(3) |
| Mean value of $d_{pp}$(A-B) = 2.67(5) | | Mean value of $d_{pp}$(A-B) = 2.70(3) | |
| $d_{pp}$* = 2.68 for **1** | | $d_{pp}$* = 2.71 for **2** | |
| Dihedral angle ($\theta$) for **1** (°) | | Dihedral angle ($\theta$) for **2** (°) | |
| $\theta$ = 7.73(1) | | $\theta$ = 10.26(7) | |
| $\sigma_{\emptyset}^2$ and $\sigma_{\alpha}^2$ for **1** | | $\sigma_{\emptyset}^2$ and $\sigma_{\alpha}^2$ for **1** | |
| $\sigma_{\emptyset}^2$ = 20.99, $\sigma_{\alpha}^2$ = 8.96 | | $\sigma_{\emptyset}^2$ = 1.55, $\sigma_{\alpha}^2$ = 4.62 | |

$\emptyset$1 = $\emptyset$(O1N2[Dy1]O5N4), $\emptyset$2 = $\emptyset$(O5N4[Dy1]O2N1), $\emptyset$3 = $\emptyset$(O2N1[Dy1]O6N3) and $\emptyset$4 = $\emptyset$(O6N3[Dy1]O1N2), in which [Dy] represents Dy used doubly with its left two atoms and its right two atoms to form two planes, for example, $\emptyset$(O1N2[Dy1]O5N4) means the dihedral angle of O1N2Dy1 plane and Dy1O5N4 plane. The $d_{pp}$(A-B) means the distance between coordination A in the upper plane and the lower plane B. $d_{pp}$* values were calculated using the program Mercury by defining the centroids of the upper and lower planes and then measuring the distances of between centroids. The $\theta$ means the dihedral angle between the upper and lower planes.

**Table S7.** Best fitted parameters obtained for the extended Debye model with ac susceptibility data from SQUID magnetometer of compound **1** under a 1000 Oe dc applied field.

| $\chi_S$ | $\chi_T$ | $\tau$ | $\alpha$ | Residual |
|---|---|---|---|---|
| 0.01947 | 0.56932 | 0.02917 | 0.05455 | 0.00547 |
| 0.01156 | 0.53641 | 0.01483 | 0.08109 | 0.00186 |
| 0.00918 | 0.49304 | 0.00745 | 0.08532 | 0.00307 |
| 0.01313 | 0.45408 | 0.0038 | 0.06633 | 0.00502 |
| 0.00749 | 0.41116 | 0.00217 | 0.09428 | 0.00128 |
| 0.00869 | 0.37611 | 0.00131 | 0.0797 | 0.00117 |
| 0.01149 | 0.35369 | 8.58386E-4 | 0.07978 | 7.79053E-4 |
| 0.00834 | 0.33272 | 5.79112E-4 | 0.10039 | 4.19364E-4 |
| 0.01379 | 0.30912 | 4.11647E-4 | 0.0889 | 2.54813E-4 |
| 0.02035 | 0.28907 | 3.02129E-4 | 0.07483 | 3.8817E-4 |
| 1.25508E-15 | 0.2617 | 1.72854E-4 | 0.08916 | 0.00101 |
| 1.74329E-15 | 0.25968 | 1.52646E-4 | 0.10813 | 2.55041E-4 |
| 2.00091E-15 | 0.24865 | 1.18321E-4 | 0.11166 | 2.57206E-4 |
| 3.08763E-15 | 0.23627 | 9.17539E-5 | 0.11636 | 5.79399E-5 |
| 5.61773E-15 | 0.22642 | 7.33018E-5 | 0.10906 | 5.22785E-5 |
| 8.57844E-15 | 0.21572 | 5.86831E-5 | 0.09752 | 3.97937E-5 |
| 2.85902E-14 | 0.20418 | 5.00007E-5 | 0.04799 | 4.91185E-5 |
| 1.44781E-14 | 0.19746 | 3.97147E-5 | 0.05882 | 3.27553E-5 |
| 2.23747E-14 | 0.18955 | 3.344E-5 | 0.0658 | 1.25681E-5 |
| 2.52677E-14 | 0.18276 | 2.76605E-5 | 0.06323 | 8.66633E-6 |
| 3.39179E-14 | 0.17734 | 2.26577E-5 | 0.08821 | 8.42287E-6 |
| | | | 0.084 (mean value) | |

**Table S8.** Best fitted parameters obtained for the extended Debye model with ac susceptibility data from SQUID magnetometer of compound **2** under a 1000 Oe dc applied field.

| $\chi_S$ | $\chi_T$ | $\tau$ | $\alpha$ | Residual |
|---|---|---|---|---|
| 0.01104 | 0.59637 | 0.06728 | 0.10027 | 0.00144 |
| 0.01166 | 0.50847 | 0.03175 | 0.0484 | 0.00178 |
| 0.01224 | 0.45649 | 0.01629 | 0.01381 | 8.22788E-4 |
| 0.00843 | 0.42761 | 0.01015 | 0.04201 | 9.4092E-4 |
| 0.01006 | 0.39058 | 0.00596 | 0.02378 | 3.84582E-4 |
| 0.00844 | 0.36031 | 0.00396 | 0.02168 | 7.73638E-4 |
| 0.01027 | 0.33908 | 0.00264 | 0.01372 | 7.53728E-4 |
| 0.00758 | 0.3195 | 0.00188 | 0.02582 | 3.39378E-4 |
| 0.00587 | 0.30338 | 0.00137 | 0.03909 | 4.96191E-5 |
| 0.00698 | 0.28864 | 0.00102 | 0.03441 | 8.40152E-5 |
| 0.00905 | 0.26894 | 7.59953E-4 | 0.01536 | 8.48753E-5 |
| 0.00737 | 0.25707 | 5.89625E-4 | 0.02513 | 4.84957E-5 |
| 0.00667 | 0.24517 | 4.63357E-4 | 0.02726 | 5.07325E-5 |
| 0.00577 | 0.23541 | 3.67732E-4 | 0.03195 | 3.97054E-5 |
| 0.00863 | 0.22482 | 2.99905E-4 | 0.02499 | 2.27902E-5 |
| 0.00438 | 0.21537 | 2.36308E-4 | 0.03763 | 1.92678E-5 |
| 0.00283 | 0.20586 | 1.90007E-4 | 0.03537 | 6.23492E-5 |
| 0.00363 | 0.1974 | 1.5551E-4 | 0.02663 | 2.72784E-5 |
| 0.00273 | 0.19022 | 1.25633E-4 | 0.03304 | 4.71783E-5 |
| 6.65748E-17 | 0.18396 | 1.00214E-4 | 0.03628 | 3.68821E-5 |
| 1.95225E-18 | 0.17752 | 8.17214E-5 | 0.03081 | 3.82762E-5 |
| 6.71521E-18 | 0.17088 | 6.53799E-5 | 0.02086 | 4.21858E-5 |
| | | | 0.031 (mean value) | |

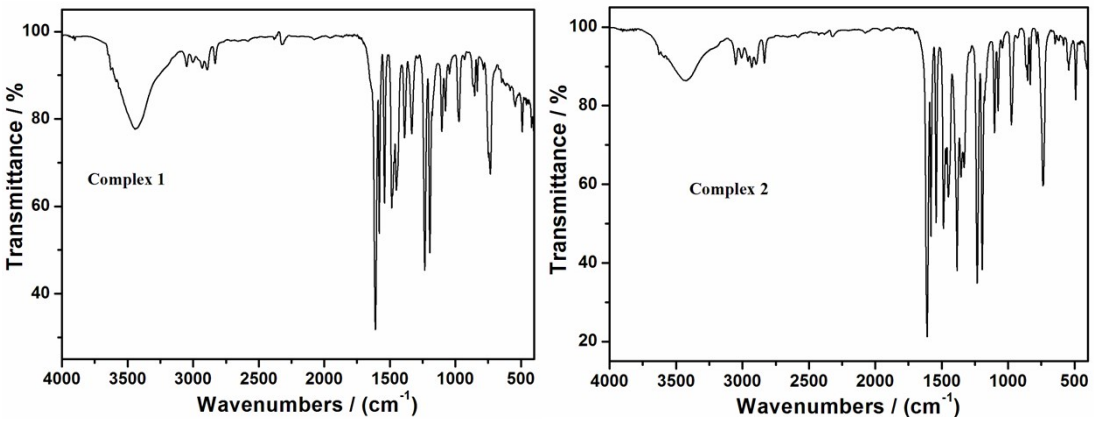


**Figure S1.** IR spectra of complexes **1** (left) and **2** (right).

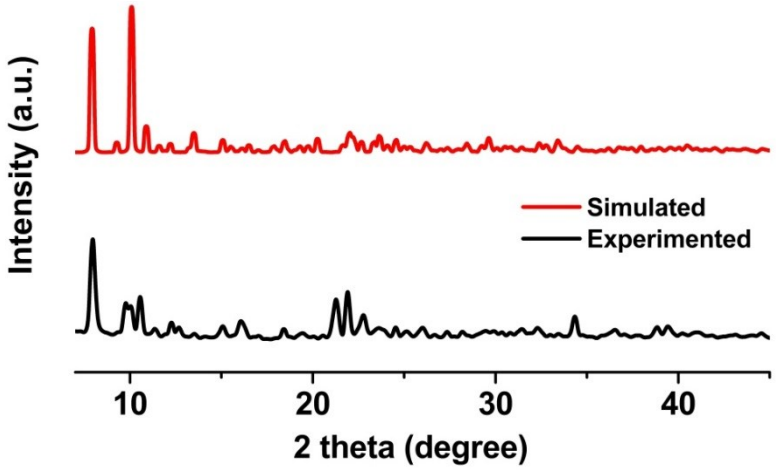


**Figure S2.** Experimental and simulated X-ray powder diffractograms for **1**.

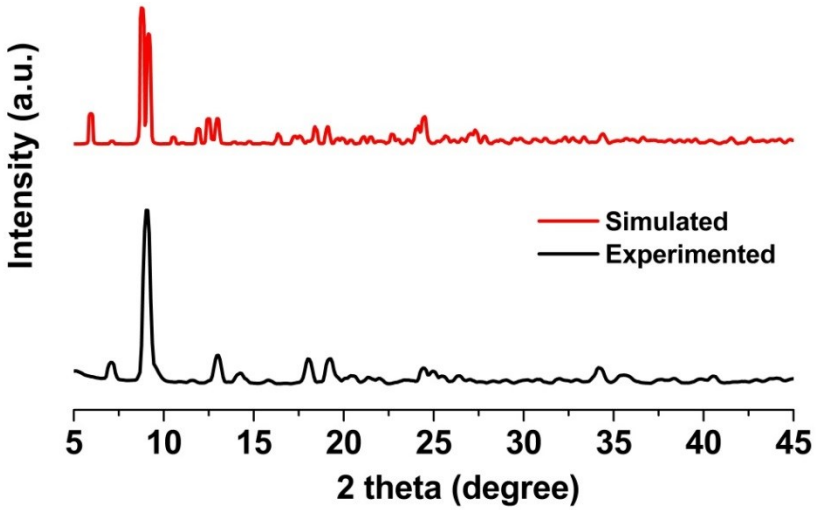


**Figure S3.** Experimental and simulated X-ray powder diffractograms for **2**.

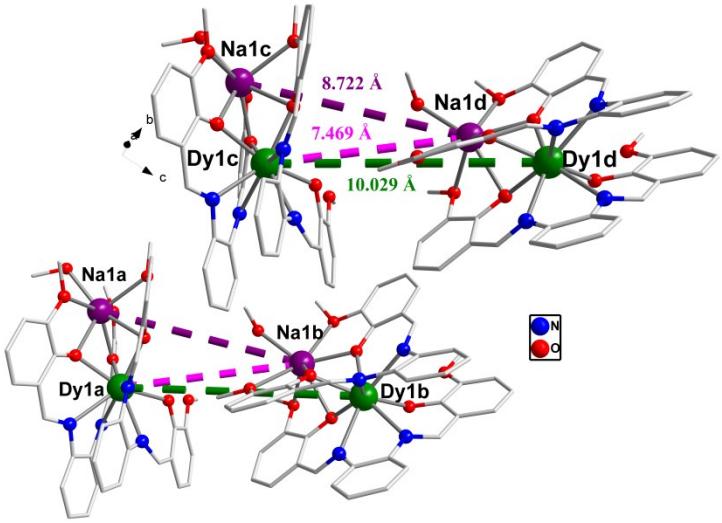


**Figure S4**. The plot showing the distances of $Na^{I}\cdots Na^{I}$ (violet), $Dy^{III}\cdots Na^{I}$ (pink) and $Dy^{III}\cdots Dy^{III}$ (green) in the crystal lattices of **1**. Symmetry codes: a (2+x, -1+y, z); b (2+x, 1.5-y, 0.5+z); c (2+x, y, z); d (2+x, 2.5-y, 0.5+z).

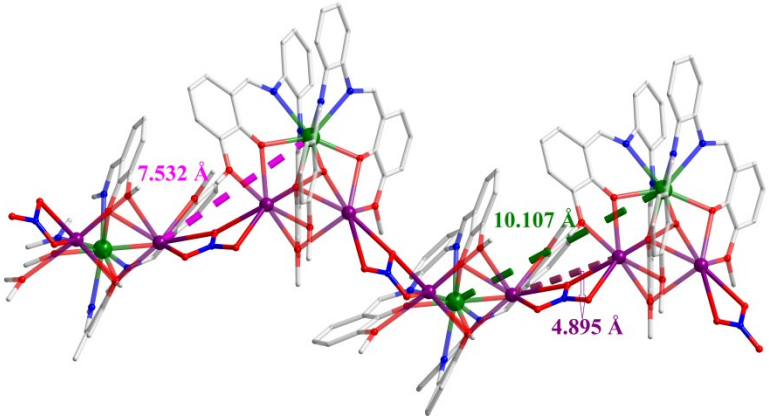


**Figure S5**. The plot showing the distances of $Na^{I}\cdots Na^{I}$ (violet), $Dy^{III}\cdots Na^{I}$ (pink) and $Dy^{III}\cdots Dy^{III}$ (green) between the neighboring $DyNa_2$ units within 1D chain of **2**.

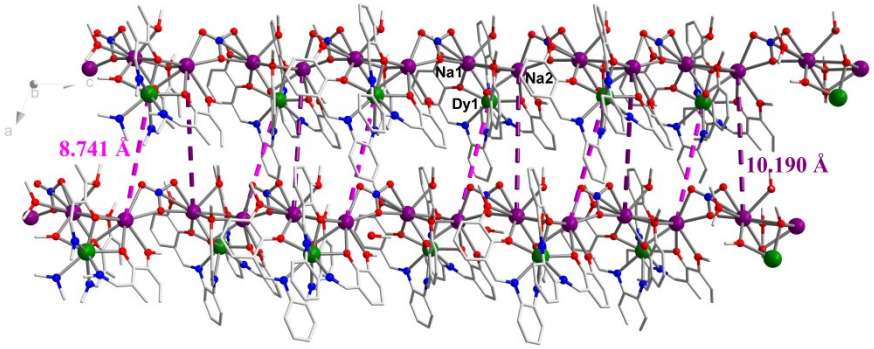


**Figure S6**. The plot showing the distances of $Dy^{III}\cdots Na^{I}$ (pink) and $Na^{I}\cdots Na^{I}$ (violet) between the 1D chains of **2**.

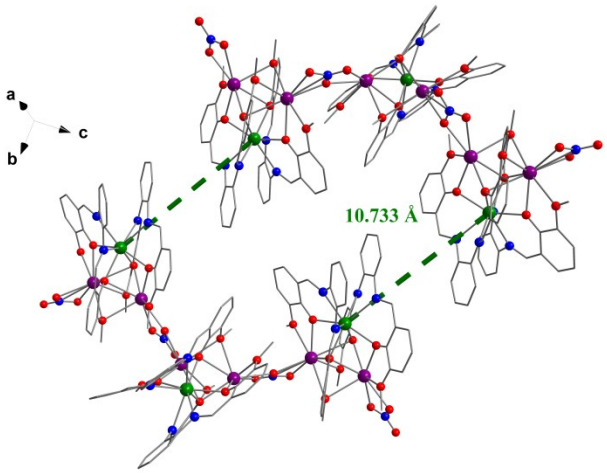


**Figure S7**. The plot showing the interchain distances of $Dy^{III}\cdots Dy^{III}$ (green) of **2**.

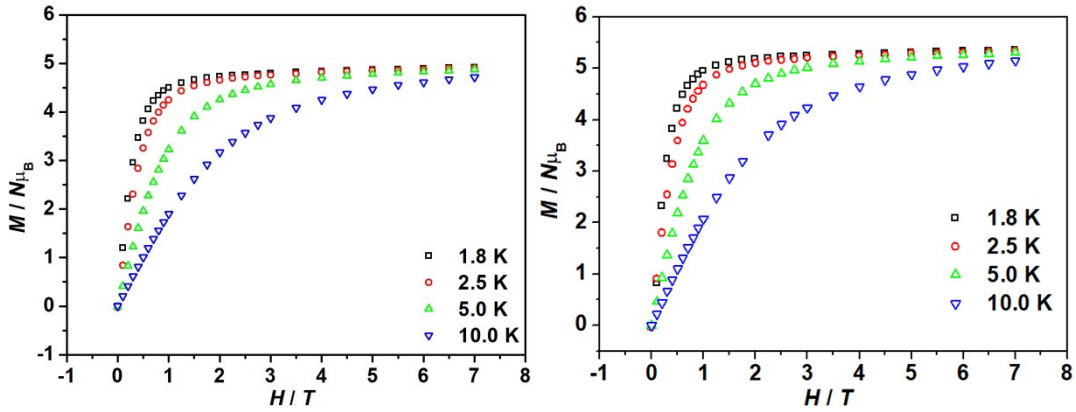


**Figure S8**. Field dependence of magnetization, *M*, at different temperature for complex **1** (left) and **2** (right).

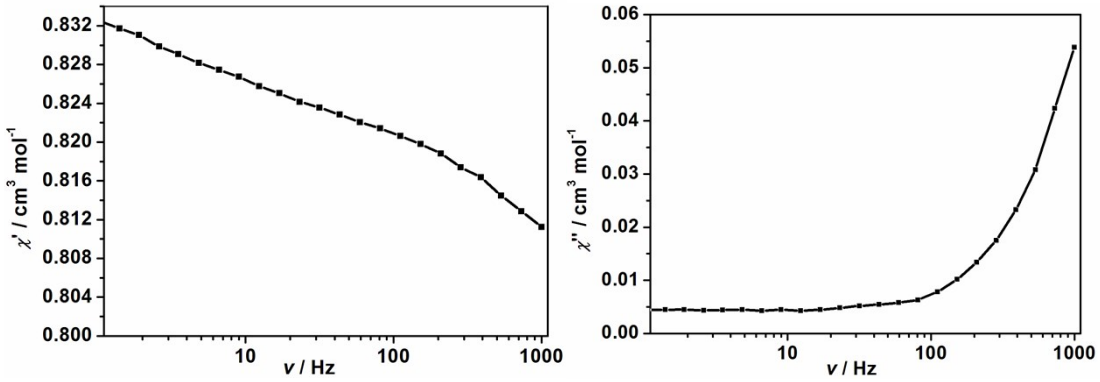


**Figure S9.** Frequency dependence of the in-phase ($\chi'$, left) and the out-of-phase ($\chi''$, right) ac signals of **1** under a zero dc field at 3.0 K.

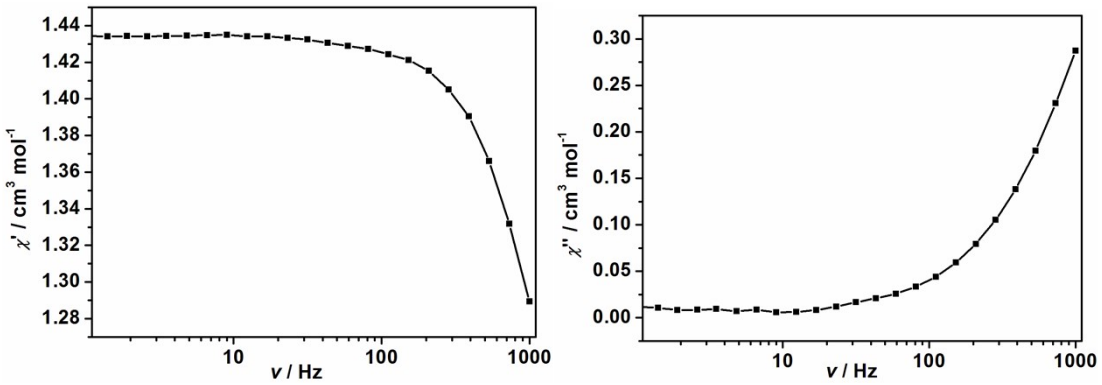


**Figure S10.** Frequency dependence of the in-phase ($\chi'$, left) and the out-of-phase ($\chi''$, right) ac signals of **2** under a zero dc field at 1.8 K.

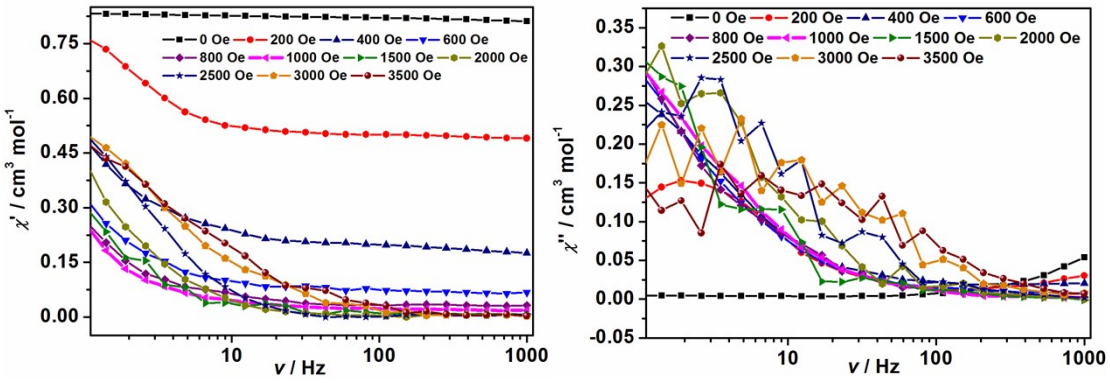


**Figure S11.** Frequency dependence of the in-phase ($\chi'$, left) and out-of-phase ($\chi''$, right) ac signals for **1** under different dc fields at 3.0 K. To see easily, the $\chi'$ and $\chi''$ ac susceptibility signals at the optimal dc field were represented by thick pink lines.

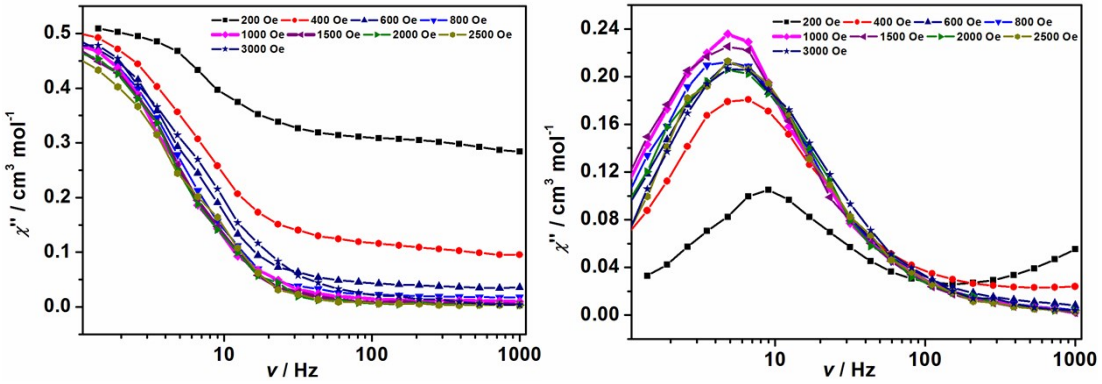


**Figure S12.** Frequency dependence of the in-phase ($\chi'$, left) and out-of-phase ($\chi''$, right) ac signals for **2** under different dc fields at 5.0 K. To see easily, the $\chi'$ and $\chi''$ ac susceptibility signals at the optimal dc field were represented by thick pink lines.

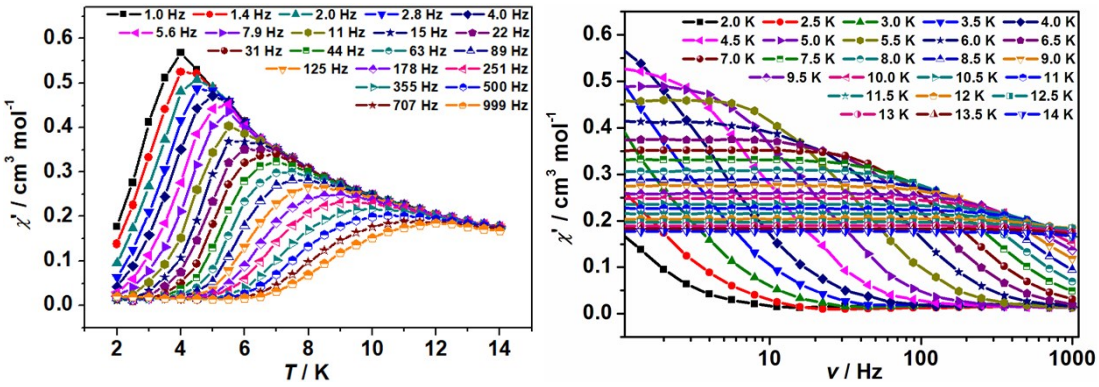


**Figure S13**. Temperature dependence (left) and frequency dependence (right) of the in-phase ($\chi'$) ac signals for **1** under a 1000 Oe dc field.

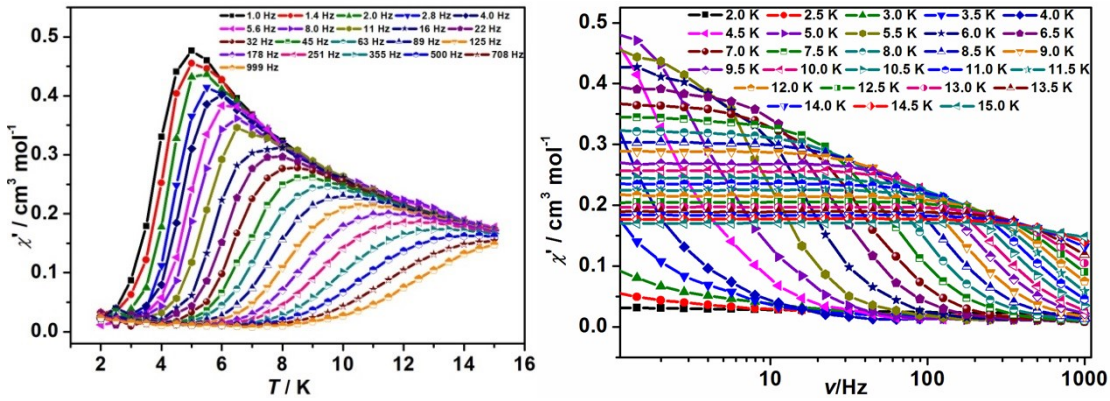


**Figure S14**. Temperature dependence (left) and frequency dependence (right) of the in-phase ($\chi'$) ac signals for **2** under a 1000 Oe dc field.

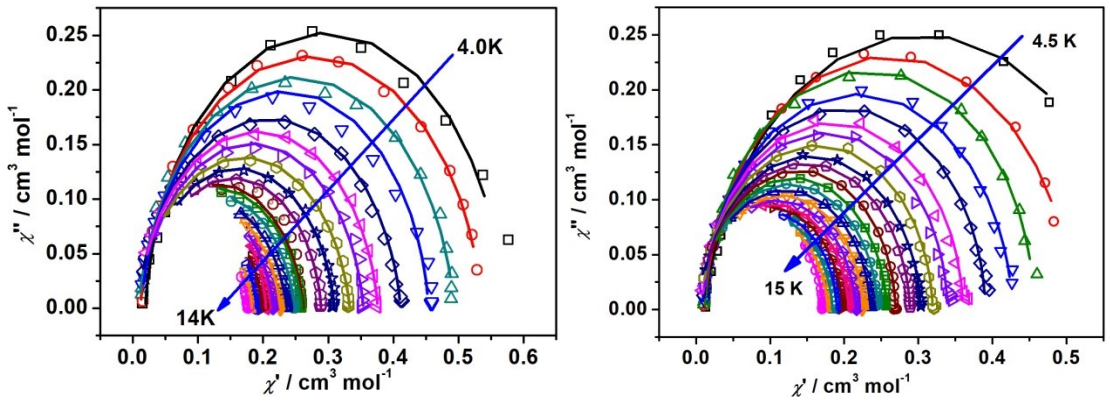


**Figure S15**. Cole-Cole plots for complex **1** (left) and **2** (right) under a 1000 Oe dc field. The solid lines represent the fitted results by using the generalized single relaxation process Debye model.

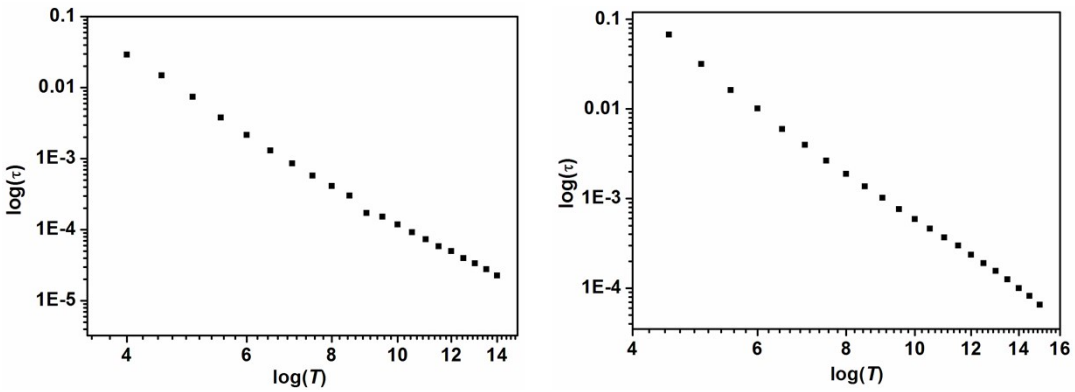


**Figure S16**. Plots of ln($\tau$) *vs*. $T^{-1}$ and log($\tau$) *vs*. log($T$) for **1** (left) and **2** (right).