

Electronic supporting information

**Slow magnetic relaxation in a lanthanide helix chain
compound $[\text{Dy}(\text{HNA})(\text{NA})_2(\text{NO}_3)]_n$**

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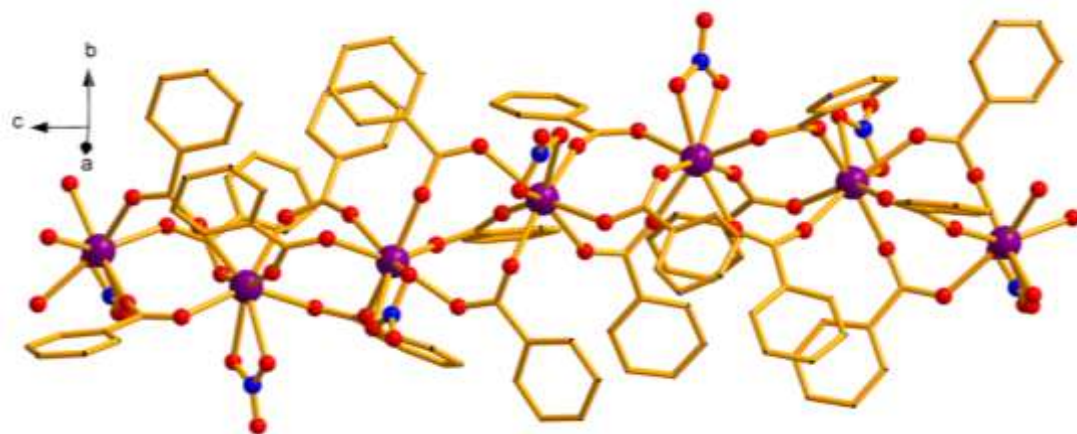


Fig. S1 1D chain structure observed in compound 1.

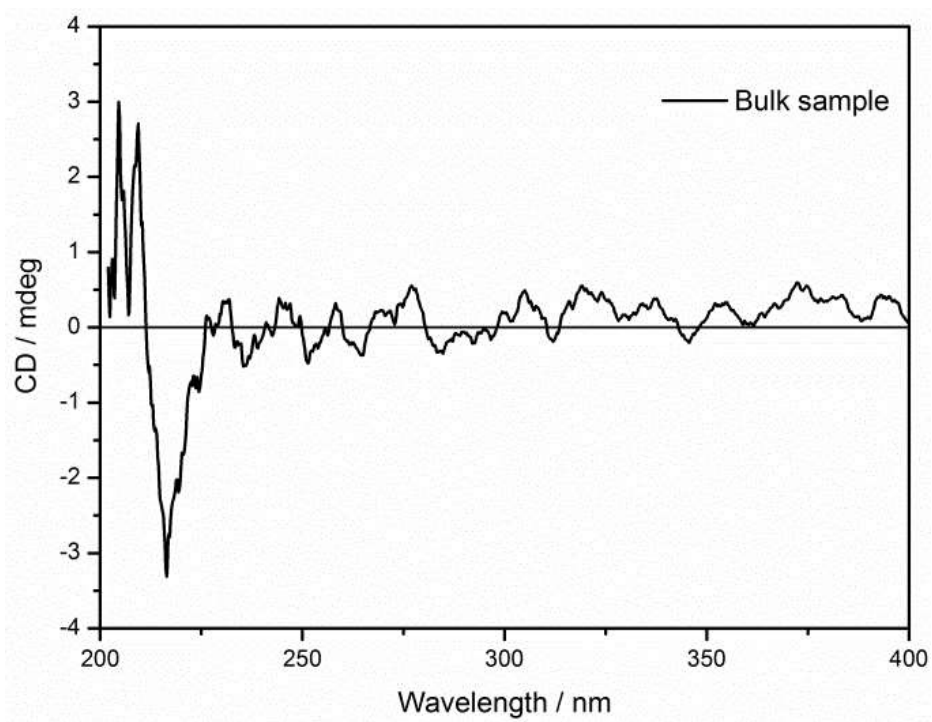


Fig. S2 Solid-state CD spectrum of 1 in bulk sample.

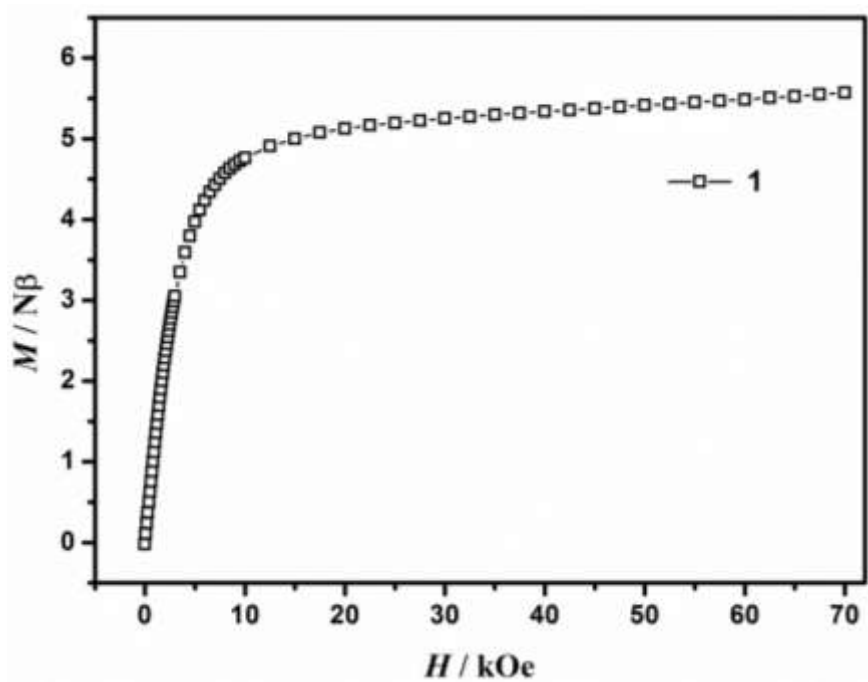


Fig. S3 Magnetization versus field of **1** at 2 K.

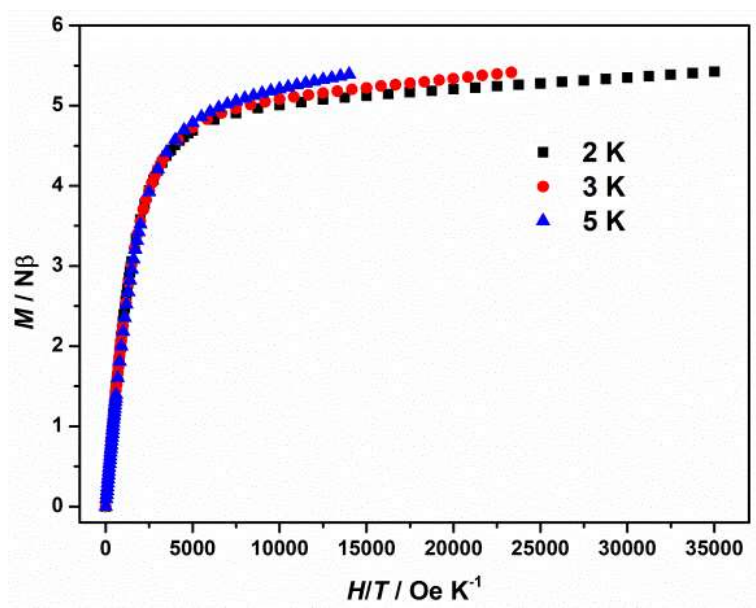


Fig. S4 Field dependence of the magnetization at different temperatures of **1**.

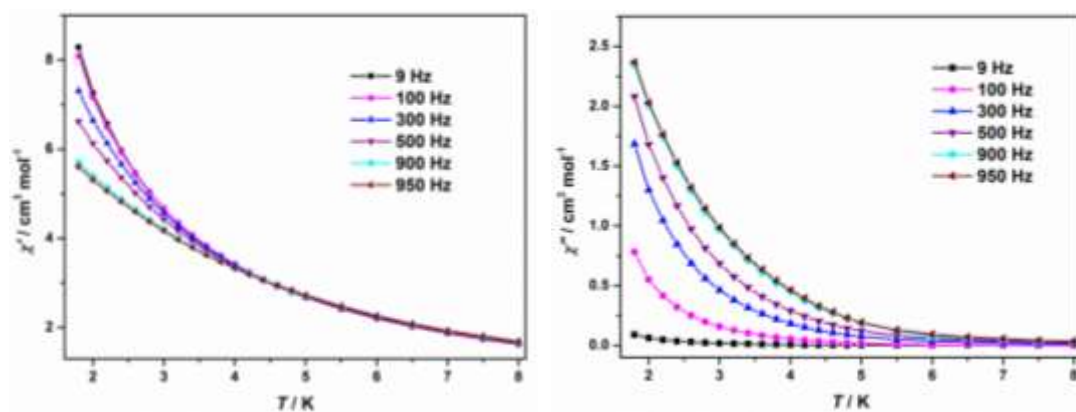


Fig. S5 Temperature dependence of in-phase and out-of-phase ac susceptibility component at different frequencies for **1** with zero dc field and an oscillation of 2.5 Oe.

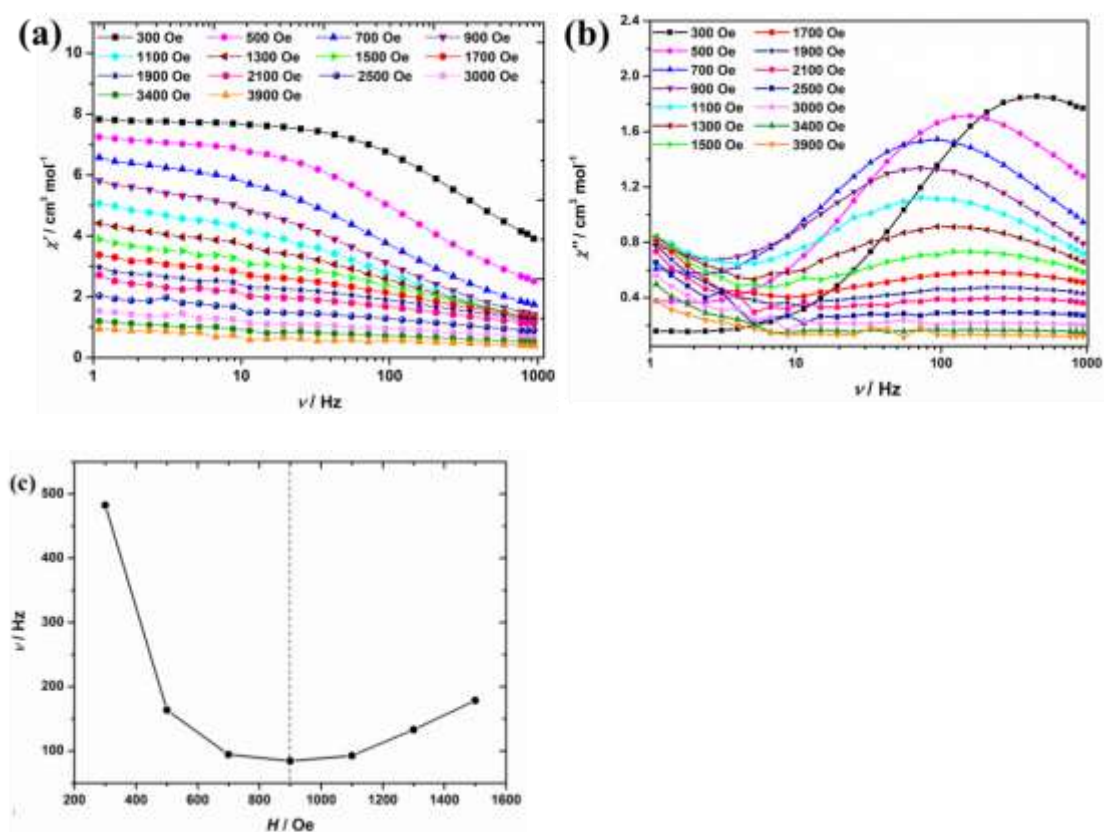


Fig. S6 Frequency dependence of the in-phase (a) and out-of-phase (χ'') (b) ac susceptibility components for **1** measured at 1.8 K with different dc fields and an oscillation of 2.5 Oe; (c) Field dependence of the frequency from χ'' vs ν data.

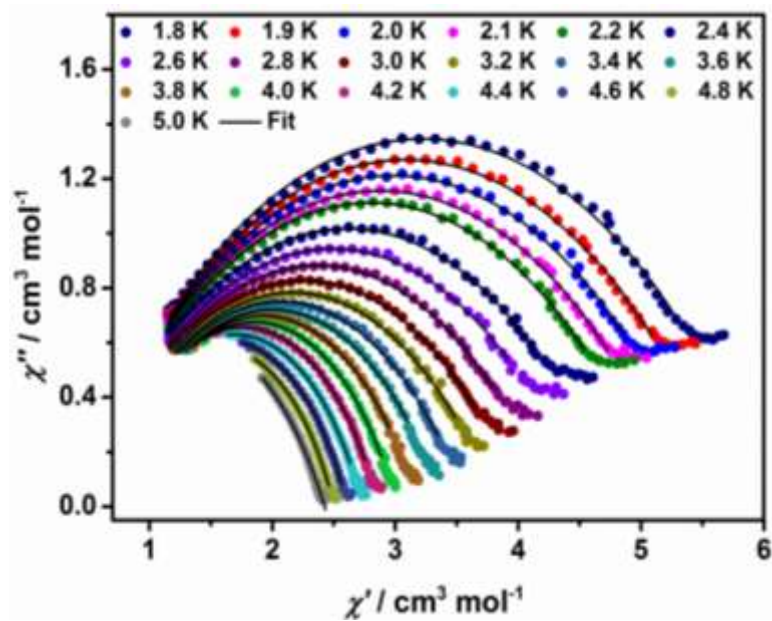


Fig. S7 Cole-Cole diagram for **1** at indicated temperatures under 900 Oe dc fields. The black lines are fitting results by Debye model.

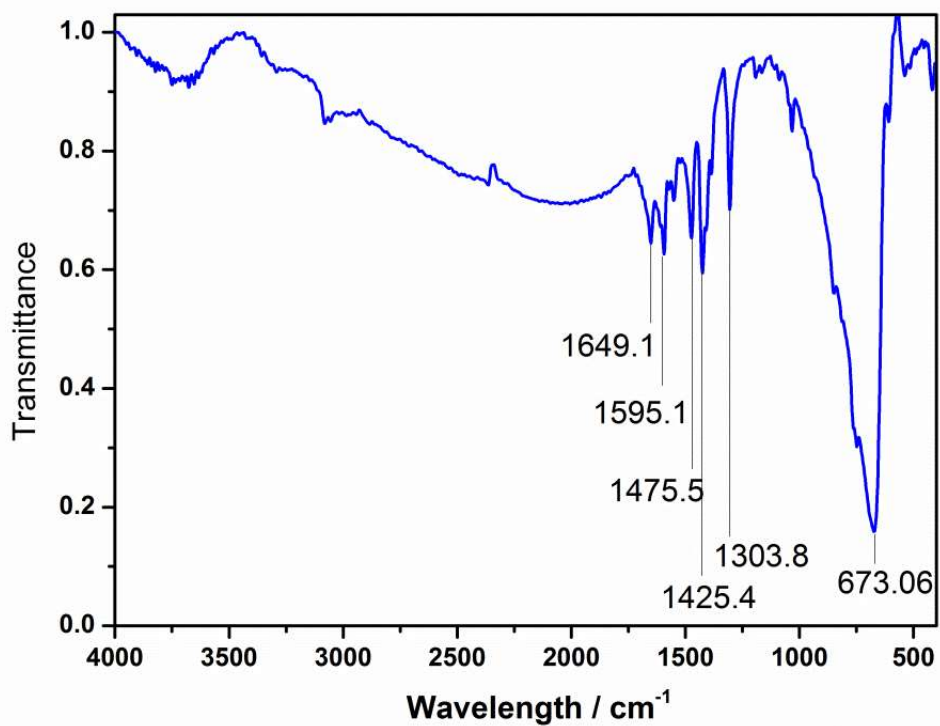


Fig. S8 The IR spectrum of compound **1**.

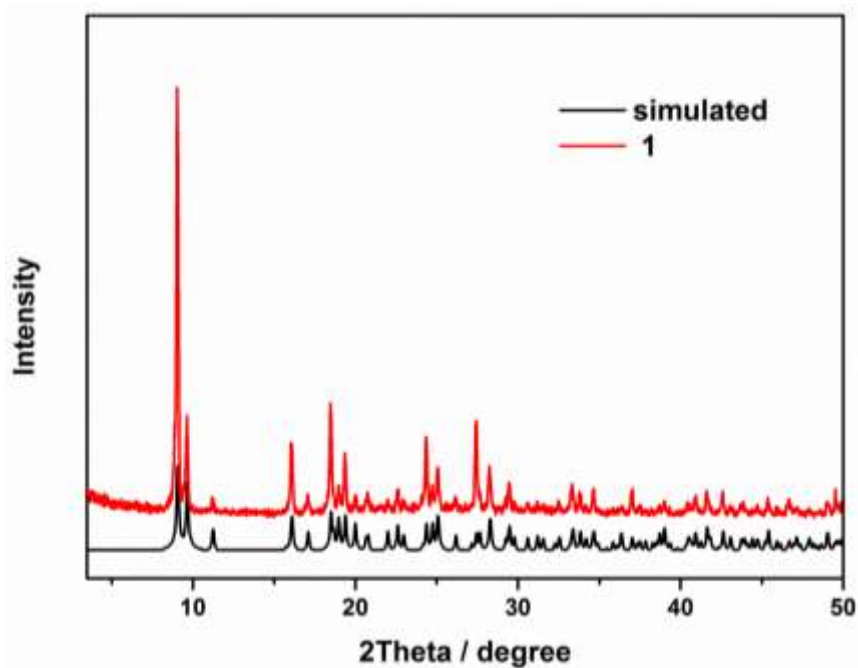


Fig. S9 Comparison of experimental and simulated powder XRD patterns of **1**.

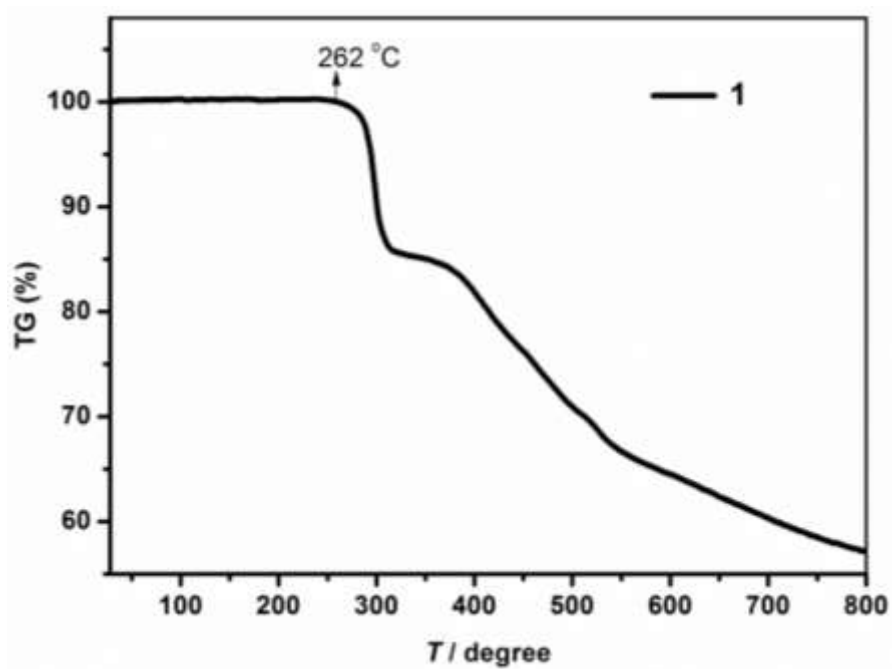


Fig. S10 There is no weight loss from room temperature to about 260 °C, corresponding to no free guest molecules in the compound. As the temperature continues to rise, dramatic weight loss occurs because of the decomposition of the organic ligands.

Table S1 Data collection and refinement for compounds **1-P6₁** and **1-P6₅**.

| Compound | 1-P6₁ | 1-P6₅ |
|---|---|---|
| CCDC no. | 1008253 | 1008252 |
| formula | C ₁₈ H ₁₃ DyN ₄ O ₉ | C ₁₈ H ₁₃ DyN ₄ O ₉ |
| M | 591.82 | 591.82 |
| Temperature (K) | 128(2) | 128(2) |
| crystal system | hexagonal | hexagonal |
| space group | <i>P6₁</i> | <i>P6₅</i> |
| <i>a</i> / Å | 11.2159(8) | 11.1993(9) |
| <i>b</i> / Å | 11.2159(8) | 11.1993(9) |
| <i>c</i> / Å | 26.5973(18) | 26.5836(18) |
| <i>α</i> / deg. | 90 | 90 |
| <i>β</i> / deg. | 90 | 90 |
| <i>γ</i> / deg. | 120 | 120 |
| <i>V</i> / Å ³ | 2897.6(3) | 2887.5(4) |
| <i>Z</i> | 6 | 6 |
| <i>D_c</i> / g cm ⁻³ | 2.035 | 2.042 |
| <i>μ</i> / mm ⁻¹ | 3.931 | 3.945 |
| <i>F</i> (000) | 1722 | 1722 |
| <i>R</i> (int) | 0.0511 | 0.0492 |
| total reflections | 5641 | 5649 |
| Unique reflections | 2249 | 2241 |
| <i>R</i> ₁ ^a [I>2σ(I)] | 0.0338 | 0.0282 |
| <i>wR</i> ₂ ^b [I>2σ(I)] | 0.0740 | 0.0530 |
| GOF | 1.041 | 1.028 |
| Flack | -0.027(18) | -0.019(15) |

Table S2 Selected bond lengths (Å) and angles for compounds **1-P6₁** and **1-P6₅**.

| 1-P6₁ | | 1-P6₅ | |
|-------------------------|----------|-------------------------|------------|
| Bonds/Angles (Å / °) | | Bonds/Angles (Å / °) | |
| Dy(1)-O(6)#1 | 2.252(7) | Dy(1)-O(5) | 2.262(6) |
| Dy(1)-O(2)#2 | 2.310(7) | Dy(1)-O(4)#1 | 2.303(6) |
| Dy(1)-O(1) | 2.393(7) | Dy(1)-O(6)#1 | 2.395(6) |
| Dy(1)-O(7) | 2.458(7) | Dy(1)-O(7) | 2.458(6) |
| Dy(1)-O(4)#2 | 2.295(7) | Dy(1)-O(1) | 2.285(6) |
| Dy(1)-O(3) | 2.350(7) | Dy(1)-O(2)#2 | 2.344(6) |
| Dy(1)-O(5) | 2.397(7) | Dy(1)-O(3) | 2.398(6) |
| Dy(1)-O(8) | 2.481(7) | Dy(1)-O(8) | 2.483(6) |
| Dy(1)-O(4)#2 | 2.295(7) | Dy(1)-O(1) | 2.285(6) |
| O(6)#1-Dy(1)-O(4)#2 | 160.1(2) | O(5)-Dy(1)-O(1) | 160.1(2) |
| O(6)#1-Dy(1)-O(2)#2 | 83.0(3) | O(5)-Dy(1)-O(4)#1 | 83.3(2) |
| O(4)#2-Dy(1)-O(2)#2 | 82.2(2) | O(1)-Dy(1)-O(4)#1 | 81.9(2) |
| O(6)#1-Dy(1)-O(3) | 100.0(3) | O(5)-Dy(1)-O(2)#2 | 99.6(2) |
| O(4)#2-Dy(1)-O(3) | 84.3(3) | O(1)-Dy(1)-O(2)#2 | 84.8(2) |
| O(2)#2-Dy(1)-O(3) | 143.8(3) | O(4)#1-Dy(1)-O(2)#2 | 143.7(2) |
| O(6)#1-Dy(1)-O(1) | 83.6(3) | O(5)-Dy(1)-O(6)#1 | 83.5(2) |
| O(4)#2-Dy(1)-O(1) | 79.0(2) | O(1)-Dy(1)-O(6)#1 | 104.8(2) |
| O(2)#2-Dy(1)-O(1) | 71.3(2) | O(4)#1-Dy(1)-O(6)#1 | 73.6(2) |
| O(3)-Dy(1)-O(1) | 73.2(2) | O(2)#2-Dy(1)-O(6)#1 | 142.68(19) |
| O(6)#1-Dy(1)-O(5) | 83.6(2) | O(5)-Dy(1)-O(3) | 84.0(2) |
| O(4)#2-Dy(1)-O(5) | 104.8(2) | O(1)-Dy(1)-O(3) | 78.7(2) |
| O(2)#2-Dy(1)-O(5) | 73.5(2) | O(4)#1-Dy(1)-O(3) | 71.41(17) |
| O(3)-Dy(1)-O(5) | 142.7(2) | O(2)#2-Dy(1)-O(3) | 72.94(19) |
| O(1)-Dy(1)-O(5) | 143.6(2) | O(6)#1-Dy(1)-O(3) | 143.9(2) |
| O(6)#1-Dy(1)-O(7) | 127.2(2) | O(5)-Dy(1)-O(7) | 126.9(2) |
| O(4)#2-Dy(1)-O(7) | 72.7(2) | O(1)-Dy(1)-O(7) | 73.0(2) |
| O(2)#2-Dy(1)-O(7) | 132.9(2) | O(4)#1-Dy(1)-O(7) | 132.80(19) |
| O(3)-Dy(1)-O(7) | 73.2(2) | O(2)#2-Dy(1)-O(7) | 73.49(19) |
| O(1)-Dy(1)-O(7) | 137.7(2) | O(6)#1-Dy(1)-O(7) | 75.13(19) |
| O(5)-Dy(1)-O(7) | 75.3(2) | O(3)-Dy(1)-O(7) | 137.5(2) |
| O(6)#1-Dy(1)-O(8) | 75.7(2) | O(5)-Dy(1)-O(8) | 75.5(2) |
| O(4)#2-Dy(1)-O(8) | 123.9(2) | O(1)-Dy(1)-O(8) | 124.2(2) |
| O(2)#2-Dy(1)-O(8) | 140.6(2) | O(4)#1-Dy(1)-O(8) | 140.9(2) |
| O(3)-Dy(1)-O(8) | 73.4(2) | O(2)#2-Dy(1)-O(8) | 73.17(19) |
| O(1)-Dy(1)-O(8) | 136.6(2) | O(6)#1-Dy(1)-O(8) | 71.71(19) |
| O(5)-Dy(1)-O(8) | 71.6(2) | O(3)-Dy(1)-O(8) | 136.40(19) |
| O(7)-Dy(1)-O(8) | 51.9(2) | O(7)-Dy(1)-O(8) | 51.80(17) |

Symmetry codes: For **1-P6₁**, #1 x-y+1,x,z+1/6; #2 y,-x+y+1,z-1/6; For **1-P6₅**, #1 x-y,x-1,z-1/6; #2 y+1,-x+y+1,z+1/6.

Table S3 The continuous symmetry measurement value calculated by *SHAPE* 2.0 for **1**.

| Dy ³⁺ | D_{2d} TDD | C_{2v} BTPR | D_{4d} SAPR |
|------------------|--------------|---------------|---------------|
| 1-p61 | 1.876 | 2.014 | 2.521 |
| 1-p65 | 1.874 | 2.022 | 2.546 |

Table S4 The parameters obtained from Cole-Cole plots of **1** using the Debye model.

| T / K | χ_1 | χ_2 | α_1 |
|-------|----------|----------|------------|
| 1.8 | 0.42 | 6.02 | 0.43 |
| 1.9 | 0.44 | 5.74 | 0.43 |
| 2.0 | 0.42 | 5.55 | 0.44 |
| 2.1 | 0.44 | 5.34 | 0.44 |
| 2.2 | 0.44 | 5.17 | 0.44 |
| 2.4 | 0.45 | 4.79 | 0.44 |
| 2.6 | 0.44 | 4.55 | 0.45 |
| 2.8 | 0.46 | 4.28 | 0.45 |
| 3.0 | 0.48 | 4.03 | 0.44 |
| 3.2 | 0.48 | 3.86 | 0.45 |
| 3.4 | 0.56 | 3.58 | 0.41 |
| 3.6 | 0.64 | 3.37 | 0.38 |
| 3.8 | 0.66 | 3.19 | 0.36 |
| 4.0 | 0.71 | 3.01 | 0.32 |
| 4.2 | 0.67 | 2.86 | 0.31 |
| 4.4 | 0.65 | 2.73 | 0.31 |
| 4.6 | 0.62 | 2.61 | 0.30 |
| 4.8 | 0.57 | 2.50 | 0.31 |
| 5.0 | 0.38 | 2.41 | 0.32 |