Cyanometallate- and carbonate-bridged dysprosium chain complex with a pentadentate macrocyclic ligand: synthesis, structure, and magnetism

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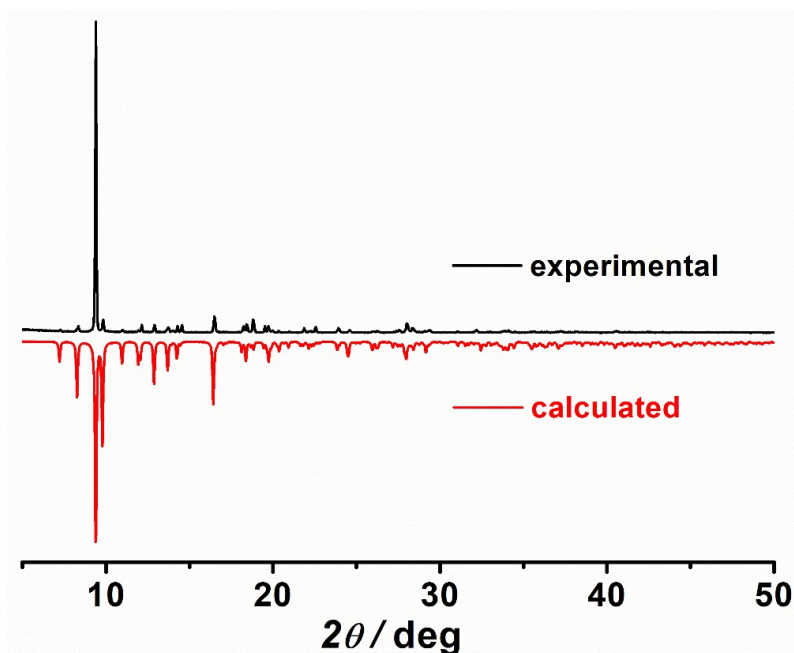
Electronic Supplementary Information

Fig. S1 PXRD pattern for complex **1**.

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

	1
Molecular formula	$C_{39}H_{51}Dy_2FeN_{16}O_4$
CCDC no	2151632
Formula weight	1188.80
Temperature	293(2) K
Wavelength / Å	0.71073
crystal system	Triclinic
Space group	P-1
a / Å	10.4443(3)
b / Å	11.0826(3)
c / Å	13.4916(4)
α / deg	97.268(2)°
β / deg	111.991(2)°
γ / deg	99.703(2)°
V / Å^3	1396.26(7)
Z	1
D_{calc}, g/cm^3	1.415
μ / mm^{-1}	2.952
F (000)	588
Goodness-of-fit on F^2	1.025
Final R indices [I >2σ(I)]^a	$R_1 = 0.0334$, $wR_2 = 0.0591$
R indices (all data)^a	$R_1 = 0.0462$, $wR_2 = 0.0615$

$^a wR_2 = [\Sigma[w(F_o{}^2-F_c{}^2)^2]/\Sigma[w(Fo^2)^2]]^{1/2}$, $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$.

**Table S2.** Continuous Shape Measure (CShM) analysis for **1**. The lowest CShM value is highlighted.

|	Octagon (D_{8h})	Heptagonal pyramid (C_{7v})	Hexagonal bipyramid (D_{6h})	Cube (O_h)	Square antiprism (D_{4d})	Triangular dodecahedron (D_{2d})	Biaugmented trigonal prism (C_{2v})
1	33.332	23.670	12.952	10.052	4.477	1.820	2.450
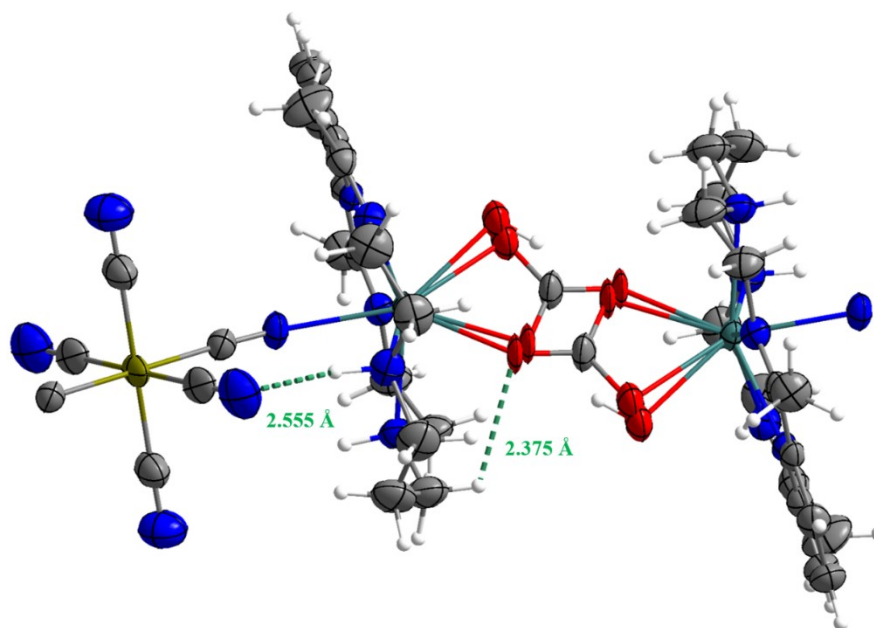
Fig. S2 The intramolecular hydrogen bonds for complex **1**.
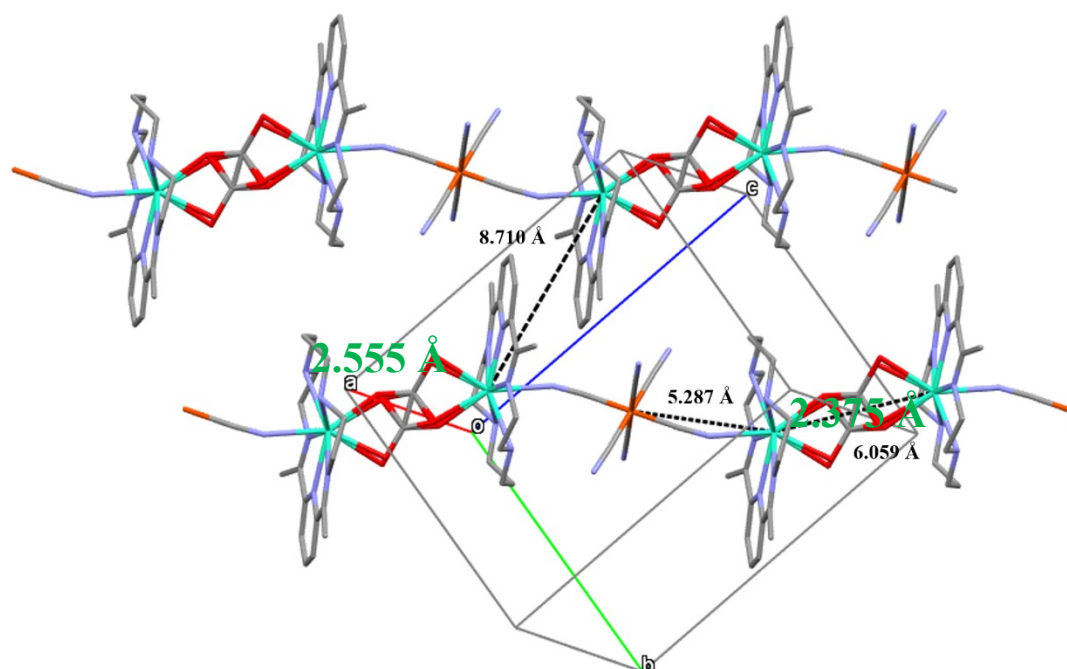
Fig. S3 Packing diagram of complex **1**. Hydrogen atoms are omitted for clarity.
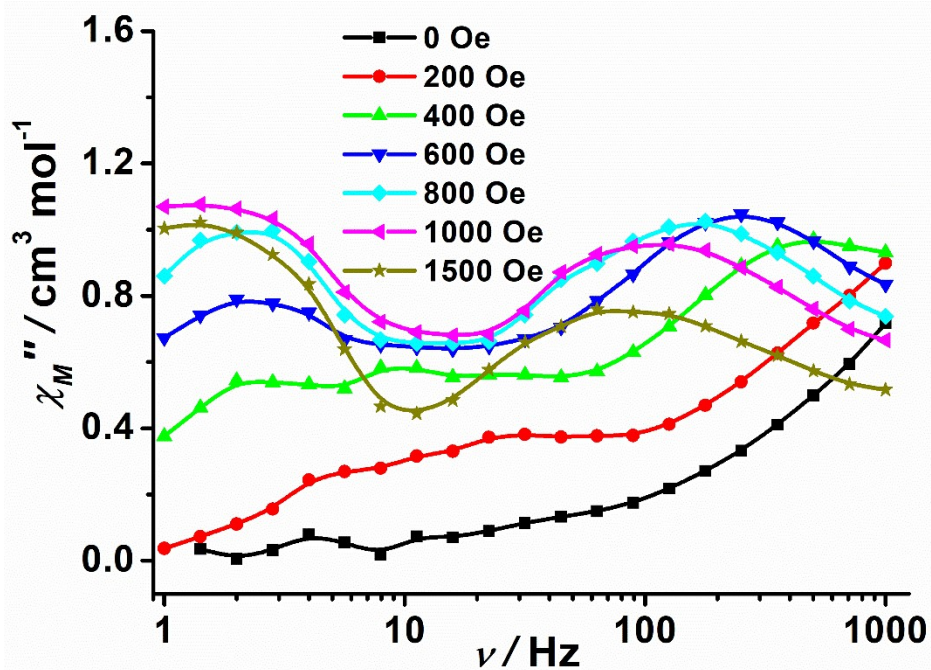
Fig. S4 Frequency dependence of out-of-phase (χ_M'') components of ac magnetic susceptibility data for **1** at 1.8 K under the applied static field from 0 to 1500 Oe. The solid lines are for eye guide.
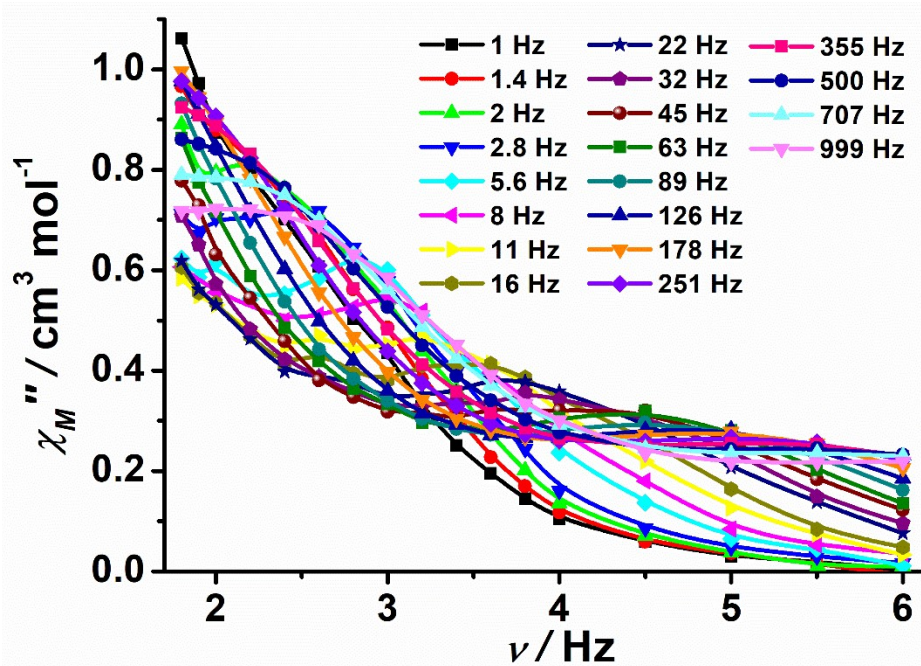
Fig. S5 Variable-temperature out-of-phase (χ_M'') components of ac magnetic susceptibility data under a dc field of 800 Oe for **1**.