Electronic supplementary information

A novel oxime-derived 3d-4f single-molecule magnet exhibiting two single-ion magnetic relaxations

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Table S1 Calculation of the agreement between the coordination polyhedron of the studied complexes with various ideal polyhedra using the SHAPE program[*]

Ideal polyhedron geometry	SAP (D_{4d})	BTPR (C_{2v})	TDD (D_{2d})
Agreement factor for Dy1	1.692	1.842	2.554
Agreement factor for Dy2	1.142	1.546	1.444

[*] SAP = Square antiprism, BTPR= Biaugmented trigonal prism and TDD = Triangular dodecahedron

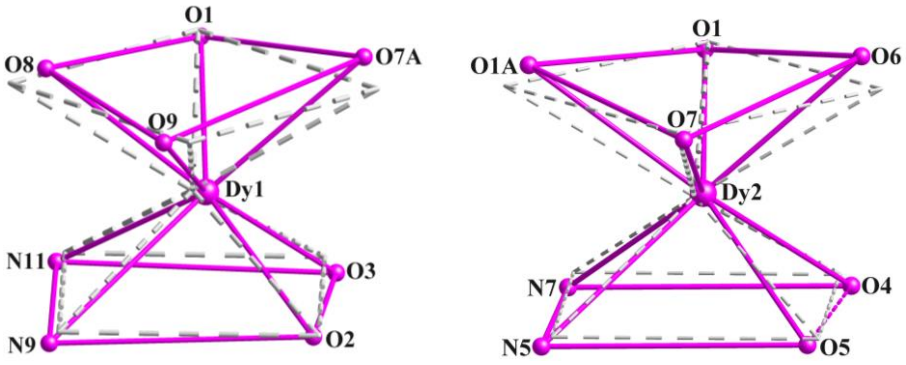

Fig. S1 Superposition diagrams of ideal square antiprism and the Dy^{III} site in **1**.

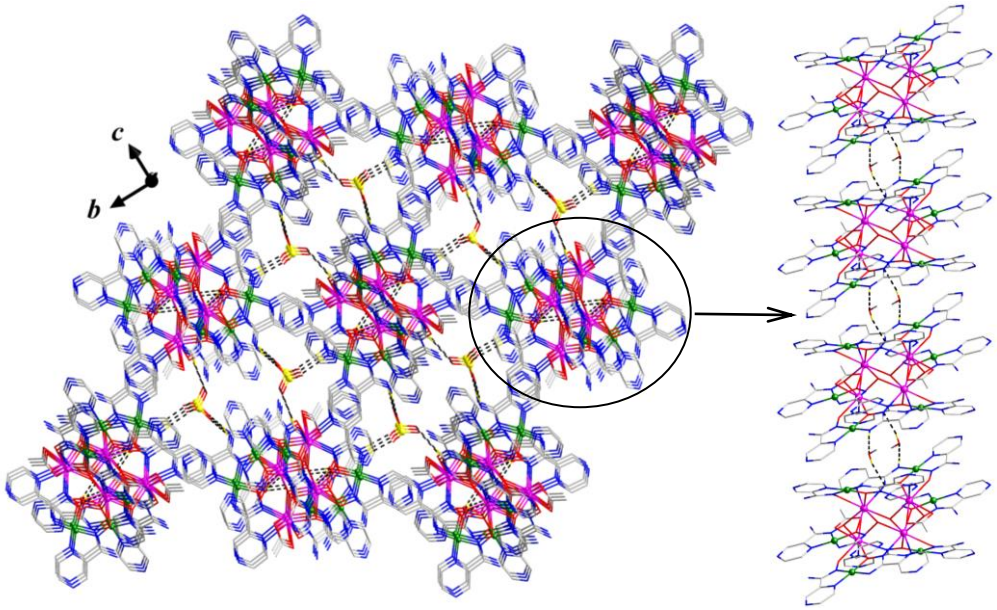

Fig. S2 3D supramolecular structure of **1** generated by intermolecular hydrogen-bonding interactions.

Table S2 Hydrogen-bonding parameters (Å, deg) in **1** [a]

D–H···A	*d* (D–H)	*d* (H···A)	*d* (D···A)	∠DHA
N(8)–H(8A)···O(14)$^{\#3}$	0.88	2.36	3.240(6)	175.8
O(14)–H(14)···N(7)$^{\#4}$	0.84	2.28	3.091(6)	163.3
N(12)–H(12A)···O(10)$^{\#1}$	0.88	2.39	3.250(7)	166.5
N(16)–H(16B)···O(12)$^{\#2}$	0.88	2.19	2.901(8)	138.0

[*] Symmetry codes: $^{\#1}$ 1 – *x*, 1 – *y*, 1 – *z*; $^{\#2}$ 1 – *x*, *y* + 1/2, 1/2 – *z*; $^{\#3}$ *x*, 1/2 – *y*, *z* + 1/2; $^{\#4}$ 1 – *x*, *y* – 1/2, 3/2 – *z*.

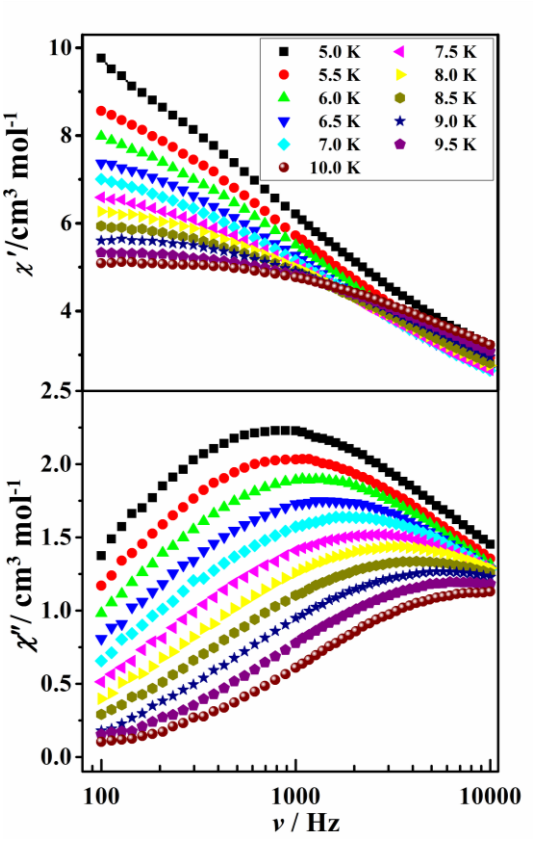

Fig. S3 Frequency dependence of the ac susceptibilities for **1** measured under H_{dc} = 0 and H_{ac} = 3.5 Oe.

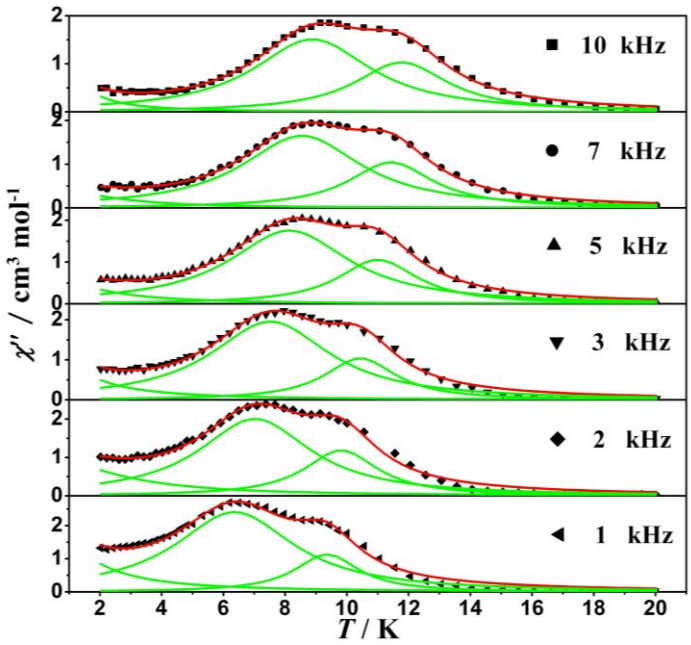

Fig. S4 Fitting of the peak position to determine the individual relaxation time for each frequency (Green and red lines represent the individual and sum of the peaks, respectively).

Table S3 Fitting results for the Cole–Cole plots of **1** under 1000 kOe dc field by using the sum of two modified Debye models

T / K	$\chi_{S,tot}$	$\Delta\chi_1$	τ_1 / s	α_1	$\Delta\chi_2$	τ_2 / s	α_2
5.0	0.46562	5.41146	4.47374E-4	0.25277	5.91834	1.82E-3	0.01984
6.0	0.38566	7.03173	3.05467E-4	0.22163	5.14239	2.35E-3	0.05238
7.0	0.37927	6.45552	1.37377E-4	0.21256	5.12681	1.84E-3	0.09032
7.2	0.37507	6.12109	1.24247E-4	0.20907	4.99070	1.76E-3	0.07971
7.6	0.38708	5.59913	8.44669E-5	0.20302	5.22188	1.36E-3	0.12481
8.0	0.37243	5.68223	5.72014E-5	0.22211	4.80010	9.09E-4	0.13273
8.5	0.36788	5.30329	3.97028E-5	0.22952	4.31512	5.95E-4	0.11735
9.0	0.33401	5.55692	2.51521E-5	0.26735	3.65907	3.44E-4	0.10815
10.0	1.07891	4.25399	1.33020E-5	0.21102	3.21132	1.25E-4	0.11290