Supporting Information for:

Dodecanuclear Heterometallic Dysprosium-Cobalt Wheel Exhibiting Single-Molecule Magnet Behaviour

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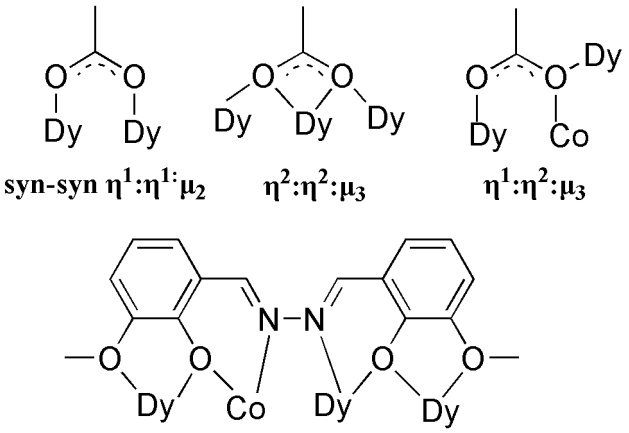
Experimental Section

Synthesis of 1: To a slurry of H_2L (0.030 g, 0.1 mmol) and triethylamine (0.014 ml, 0.1 mmol) in acetonitrile (20 mL), solid $Dy(SCN)_3 \cdot 6H_2O$ (0.045 g, 0.1 mmol) was added. After stirring for 3 h, $Co(OAc)_2 \cdot 4H_2O$ (0.025 g, 0.1 mmol) was added to the resulting yellow solution. Then the mixture was stirred for another 3 h, followed by filtration. X-ray quality green rectangular crystals of 1 were formed after two weeks. Yield: 15 mg (30%, based on Dy). Elemental analysis Calcd (%) for $C_{114}H_{138}Co_4Dy_{10}N_{22}O_{62}S_{10}$: C, 27.42; H, 2.76; N, 6.17. Found: C, 26.53; H, 2.41; N, 6.35. IR (KBr, cm^{-1}): 3382(w), 2930(w), 2704(s), 1613(s), 1467(s), 1348(w), 1294(m), 1221(m), 1102(w), 1026(w), 961(w), 856(w), 778(w),649(w), 545(w) and 450(w).

X-ray Crystallography

Crystal data for **1**: $C_{114}H_{138}Co_4Dy_{10}N_{22}O_{62}S_{10}$, M_r = 4989.78, triclinic, space group $P\bar{1}$, a = 17.1089(17) Å, b = 17.1317(9) Å, c = 18.7454(9) Å, α = 115.646(1), β = 105.043(1), γ = 92.992(1), V = 4697.1(6) $Å^3$, Z = 1, D_c = 1.764 g cm^{-3}, R_{int} = 0.0256, 24174 reflections collected, R_1 (wR_2) = 0.0456 (0.1345) and S = 1.022 for 12791 observed reflections out of 16536 unique reflections with $I > 2\sigma(I)$. Crystallographic data were collected at a temperature of 191(2) K on a Bruker ApexII CCD diffractometer with graphite monochromated Mo Kα radiation (λ = 0.71073 Å). Data processing was accomplished with the SAINT processing program. The structure was solved by the direct methods and refined on F^2 by full-matrix least squares using SHELXTL97. The locations of metal atoms were easily determined, and O, N and C atoms were subsequently determined from the difference Fourier maps. All non-hydrogen atoms were refined with anisotropic thermal parameters.



Scheme S1 Top: Bridging modes of the acetate groups in compound **1**. Bottom: Binding mode of L^{2-} in compound **1.**

Table S1 Bond valence sum calculations for compound **1**

Atom	Co^{II}	Co^{III}
Co1	2.5376	2.5600
Co2	3.1421	3.1461

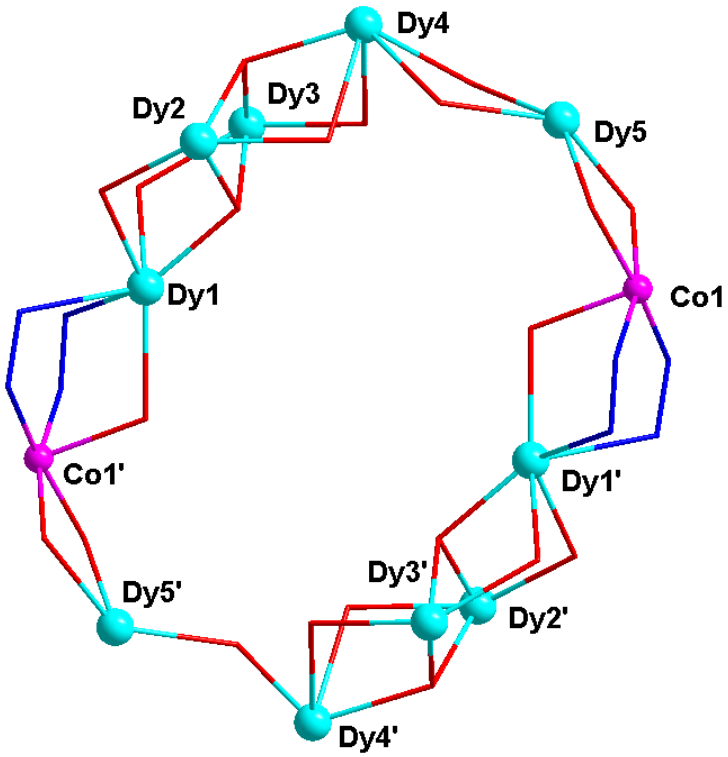


Fig. S1 Linkage of two $[Dy_5Co(\mu_3\text{-}OH)_2]^{15+}$ subcores forming the $Dy_{10}Co_2$ wheel.

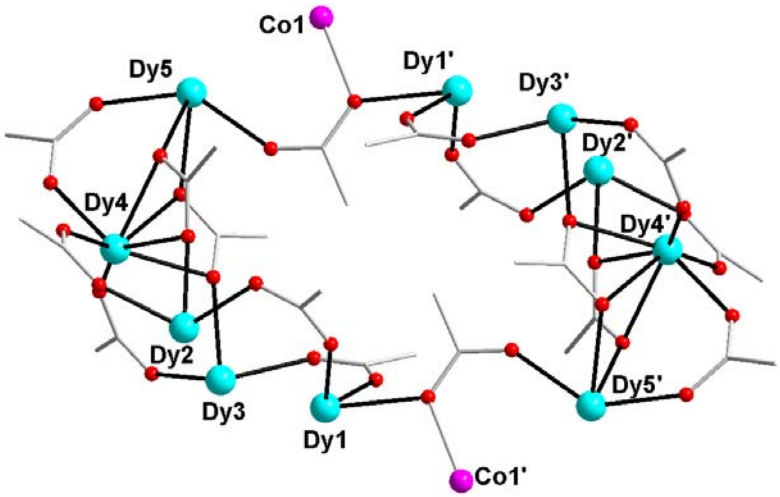


Fig. S2 Ten Dy^{III} and two Co^{II} ions bridged by sixteen acetate groups.

Magnetic measurements were performed in the temperature range 1.9 –300 K, using a Quantum Design MPMS-XL SQUID magnetometer equipped with a 7 T magnet. The diamagnetic corrections for the compounds were estimated using Pascal's constants, and magnetic data were corrected for diamagnetic contributions of the sample holder.

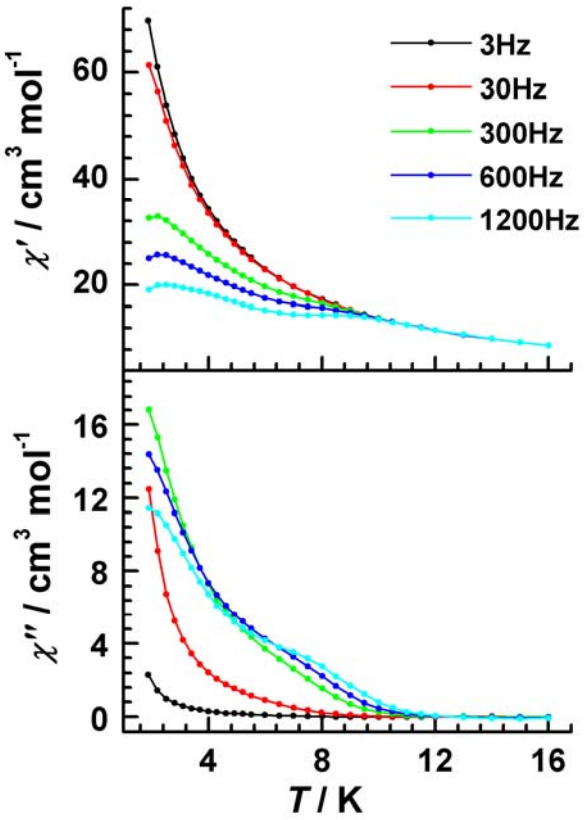


Fig. S3 Temperature dependence of the in-phase (top) and out-of-phase (bottom) ac susceptibility of **1** under zero dc field.

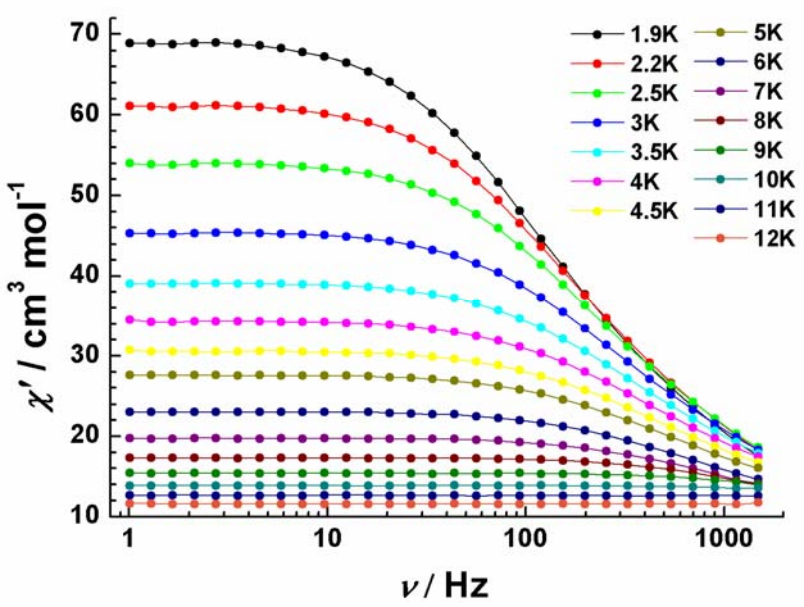


Fig. S4 Frequency dependence of the in-phase ac susceptibility of **1** below 12 K, under zero-dc field.

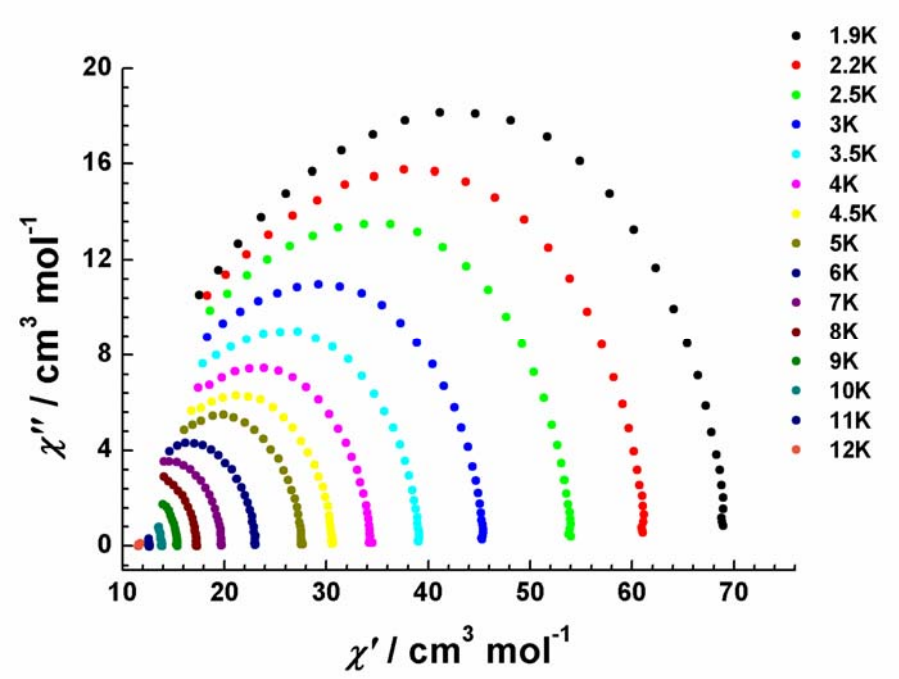


Fig. S5 Cole-Cole plots measured below 12 K and zero-dc field.

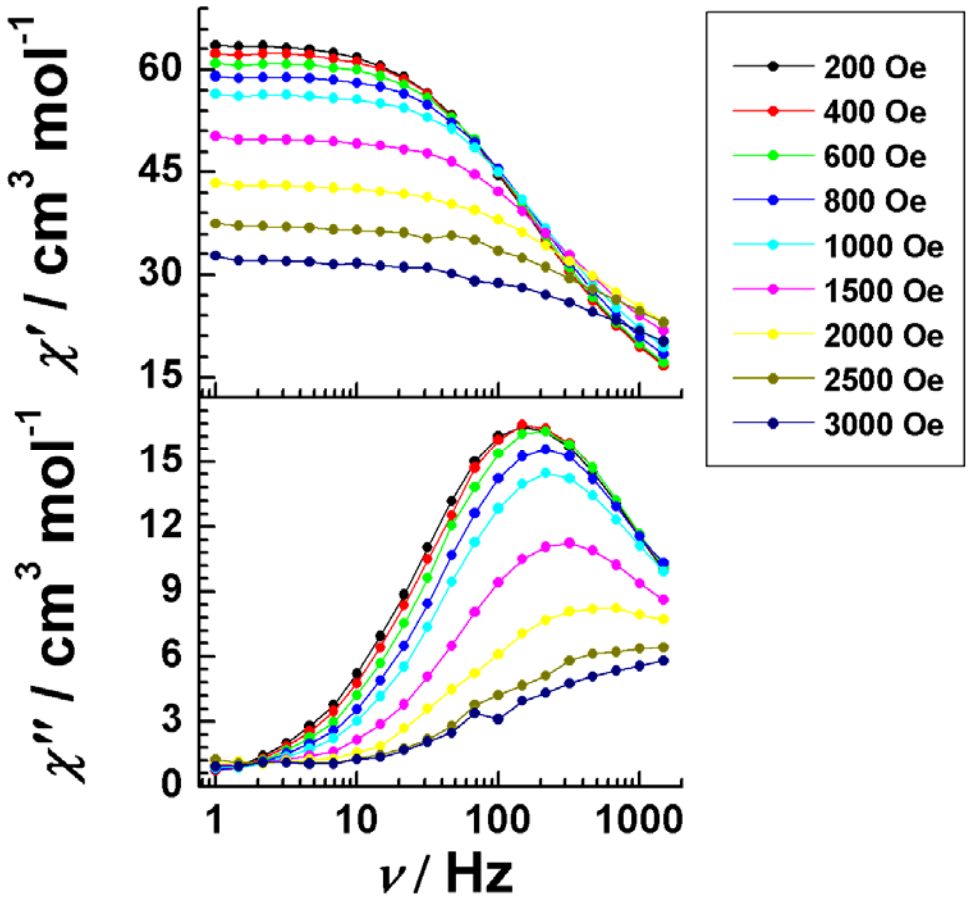


Fig. S6 The in-phase (top) and the out-of-phase (bottom) ac susceptibility as a function of the dc applied field measured at 1.9 K for **1**.

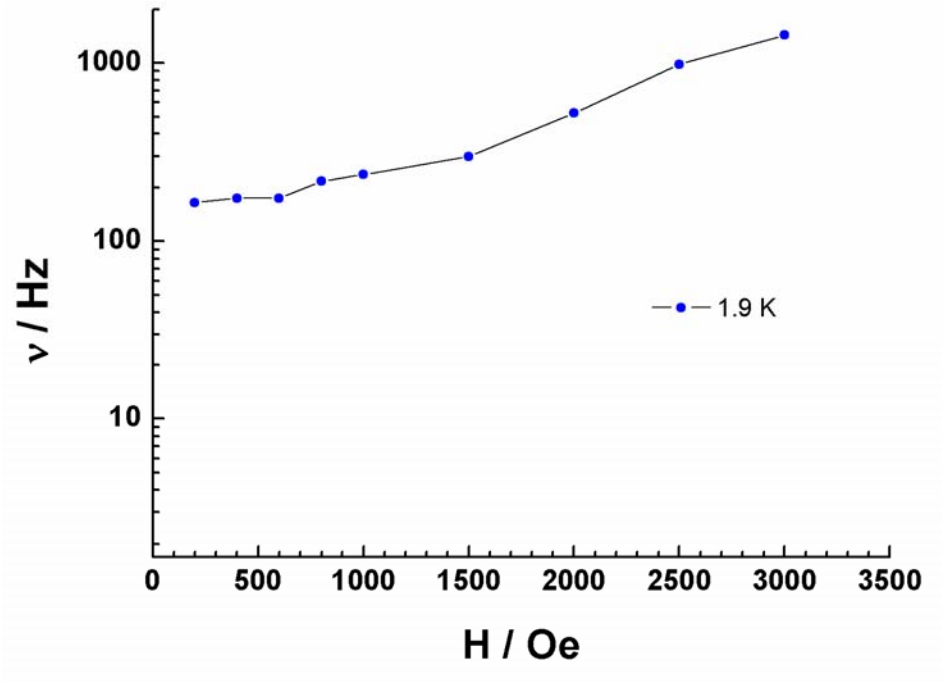


Fig. S7 Field dependence of the characteristic frequency as a function of the applied dc field for **1** at 1.9 K.

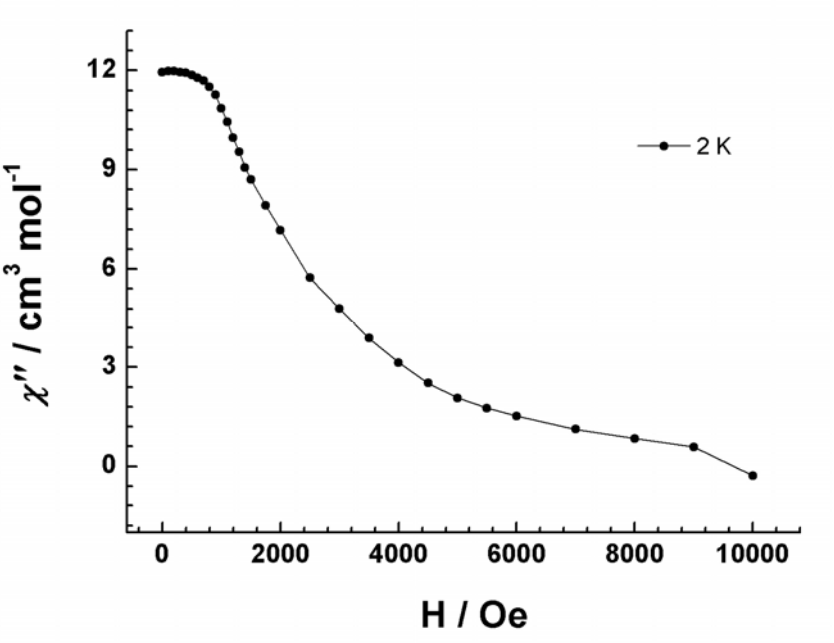


Fig. S8 Field dependence of out-of-phase ac susceptibility of **1** at 1000 Hz and 2 K.