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Supporting Information

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A Polynuclear Lanthanide Single-Molecule Magnet with a Record Anisotropic Barrier**

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Experimental part:

X-ray

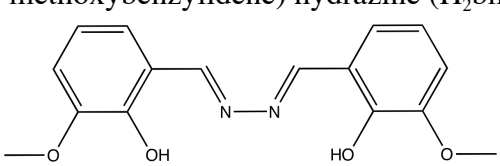
Crystals of $[C_{64}H_{66}Cl_2Dy_4N_{12}O_{18}]$ were grown from a mixture of DMF and CH_2Cl_2. A single orange block suitable for X-ray diffraction measurements was mounted on a glass fiber. Unit cell measurements and intensity data collections were performed on a Bruker-AXS SMART 1 k CCD diffractometer using graphite monochromatized Mo K_α radiation (λ = 0.71073 Å). The data reduction included a correction for Lorentz and polarization effects, with an applied multi-scan absorption correction (SADABS).

The crystal structure was solved and refined using the SHELXTL program suite. Direct methods yielded all non-hydrogen atoms which were refined with anisotropic thermal parameters. All hydrogen atom positions were calculated geometrically and were riding on their respective atoms. The largest residual electron density peak (1.580 e/Å^3) was associated with the Dy2 atom. Full-matrix least-squares refinement on F^2 gave $R_1 = 0.0491$ and $wR_2 = 0.1066$ at convergence.

Magnetism

The magnetic susceptibility measurements were obtained with the use of a Quantum Design SQUID magnetometer MPMS-XL housed at the chemistry department, University of Ottawa. This magnetometer works between 1.8 and 400 K for dc applied fields ranging from -7 to 7 T. Measurements were performed on a polycrystalline samples of 10.23 for **1**. *M vs. H* measurements has been performed at 100 K to check for the presence of ferromagnetic impurities that has been found absent. ac susceptibility measurements have been measured with an oscillating ac field of 3 Oe and ac frequencies ranging from 1 to 1500 Hz. The magnetic data were corrected for the sample holder and the diamagnetic contributions.

1,2-Bis(2-hydroxy-3-methoxybenzylidene) hydrazine (H_2bmh) :



3-methoxysalicylaldehyde hydrazone (Hmsh):

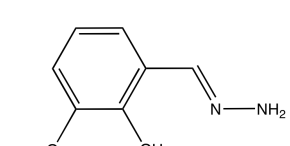


Figure S1: Schiff base ligands used for the preparation of $[Dy_4(\mu_3\text{-}OH)_2(bmh)_2(msh)_4Cl_2]$.

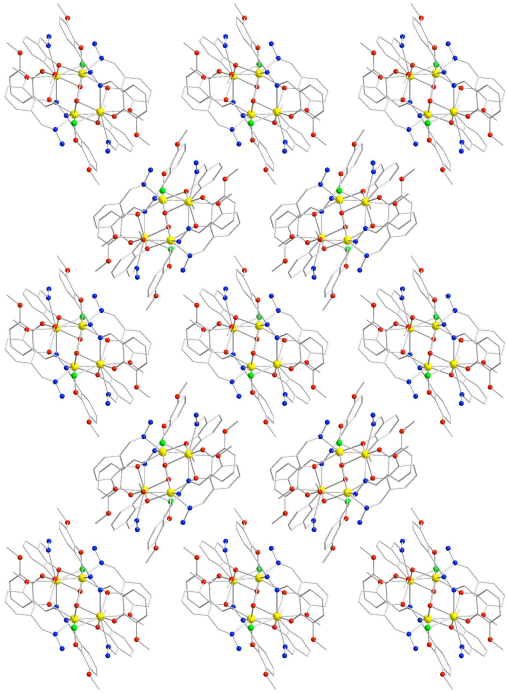


Figure S2: Zigzag packing arrangement of the molecules along *a* axis. Yellow (Dy), Red (O), Blue (N), Green (Cl).

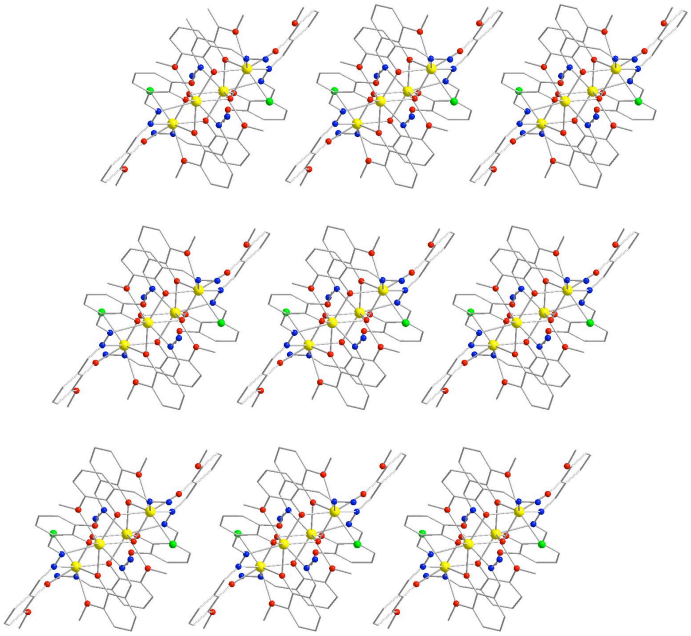


Figure S3: Packing arrangement of the molecules along *b* axis. Yellow (Dy), Red (O), Blue (N), Green (Cl).

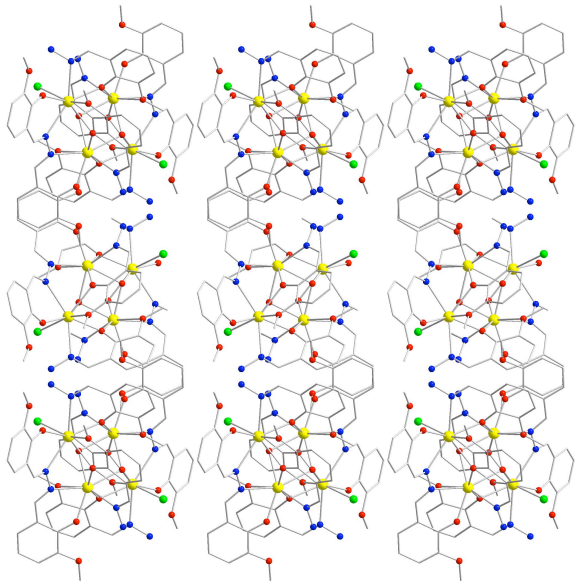


Figure S4: Packing arrangement of the molecules along *c* axis. Yellow (Dy), Red (O), Blue (N), Green (Cl).

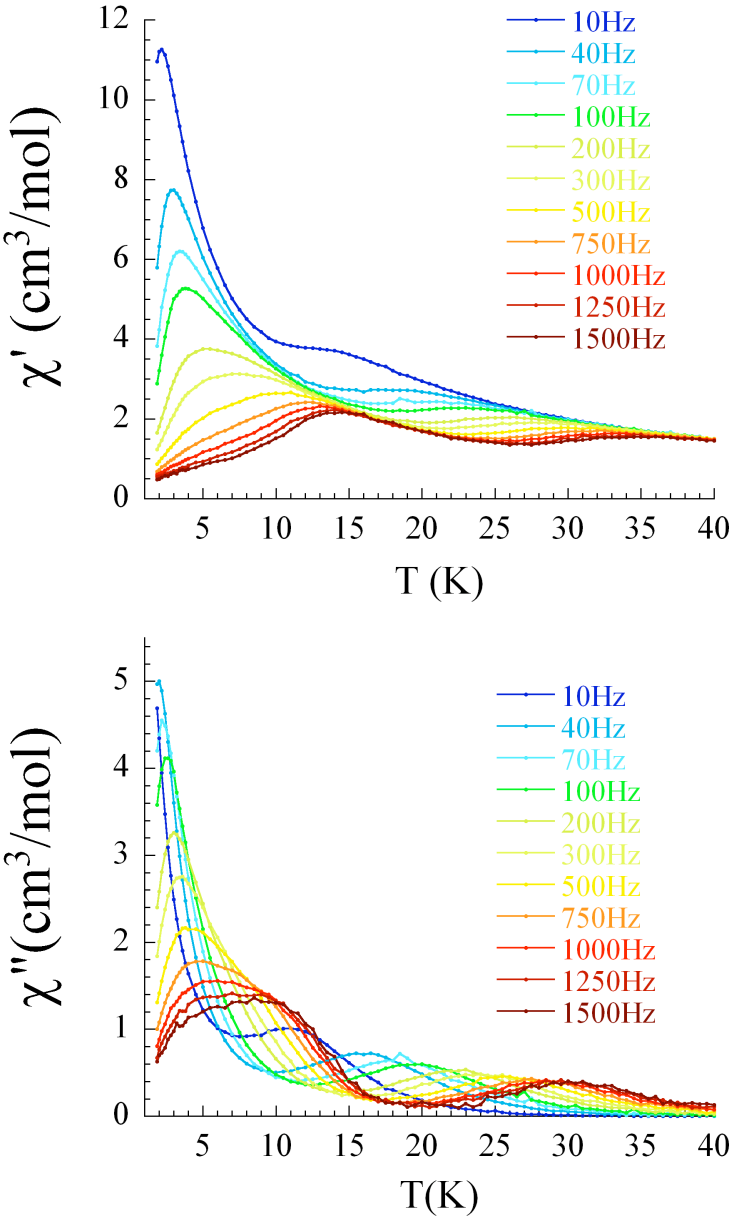


Figure S5: In-phase (χ', top) and out-of-phase (χ'', bottom) dynamic susceptibility of **1** at indicated frequencies. Solid lines are eye guides.

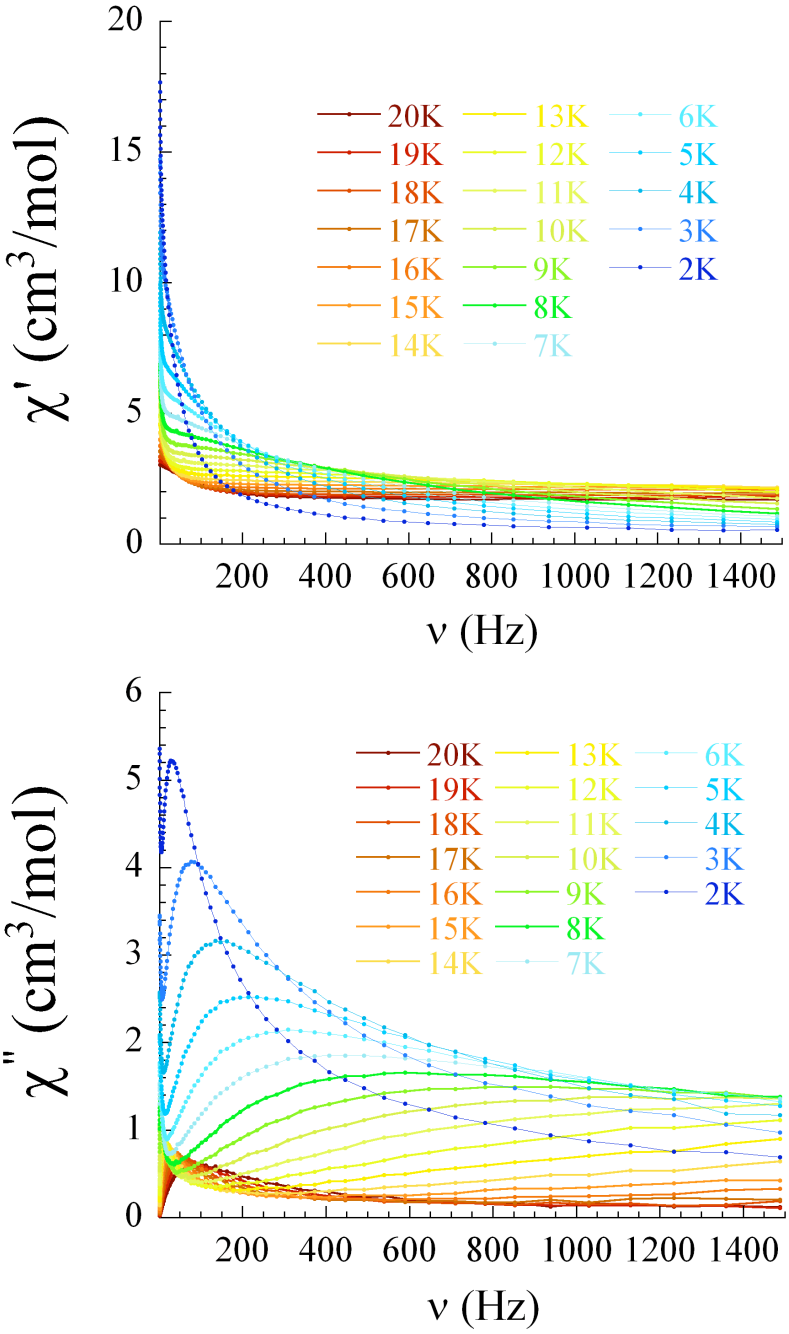


Figure S6: Frequency dependence of the in-phase (χ', top) and out-of-phase (χ'', bottom) ac susceptibility of **1** from 20 K to 2 K under zero dc field.

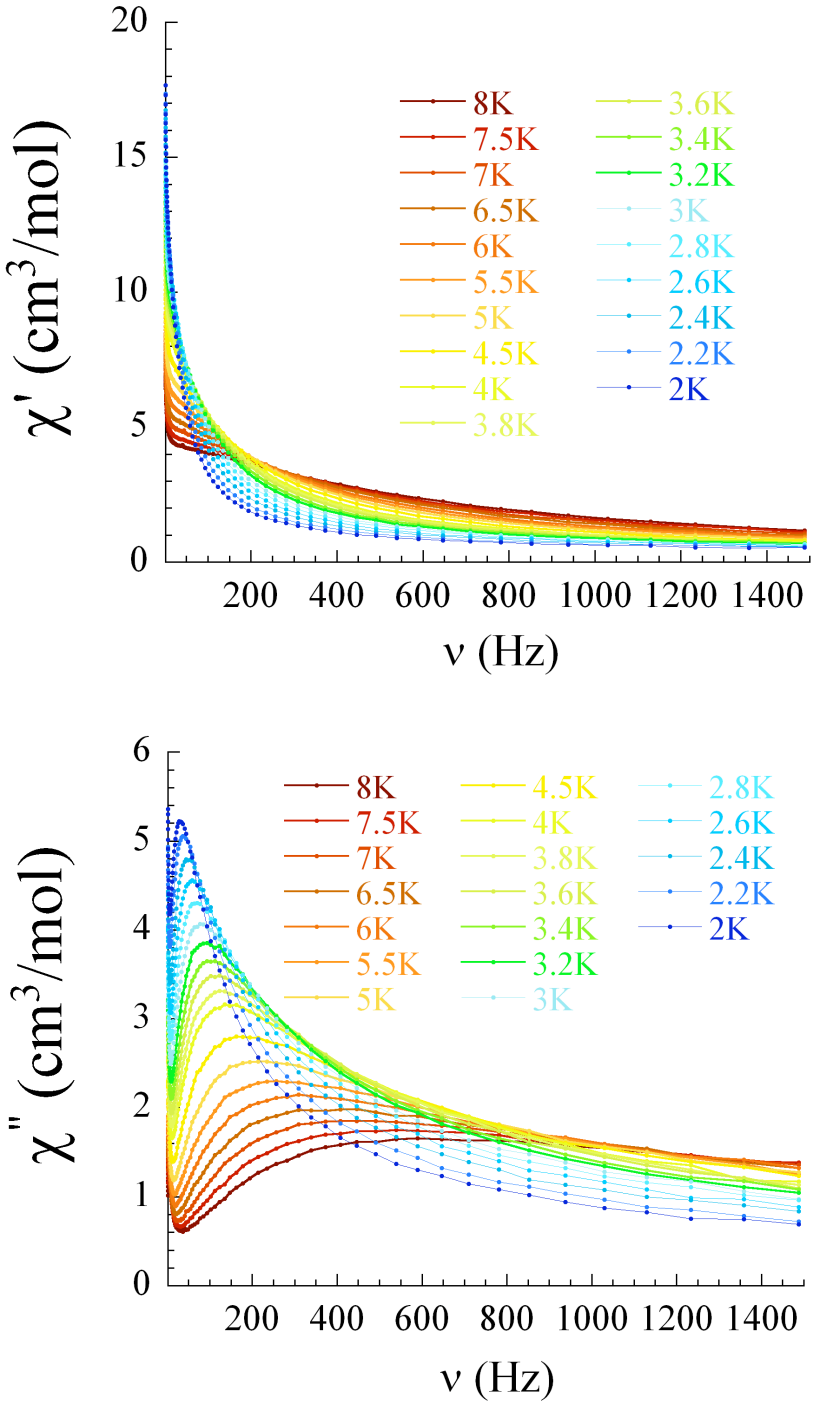


Figure S7: Frequency dependence of the in-phase (χ', top) and out-of-phase (χ'', bottom) ac susceptibility of **1** from 8 K to 2 K under zero dc field.

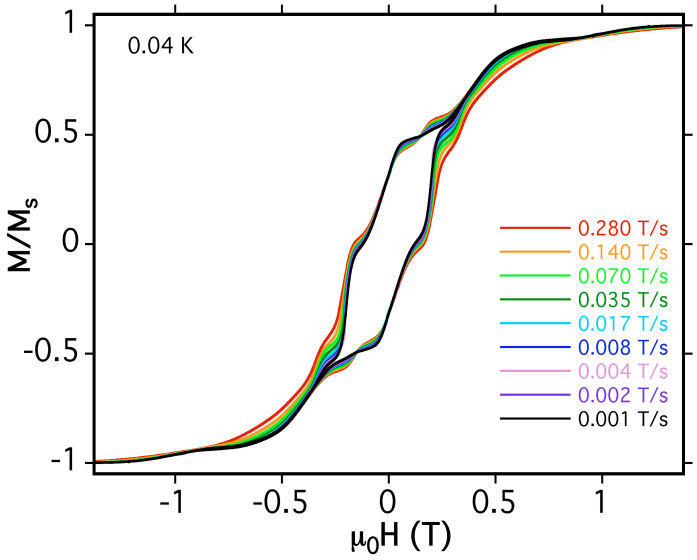


Figure S8: Magnetization (M) *vs*. applied dc field sweeps at the indicated sweep rates and at 0.04 K. M is normalized to its saturation value, Ms, at 1T.

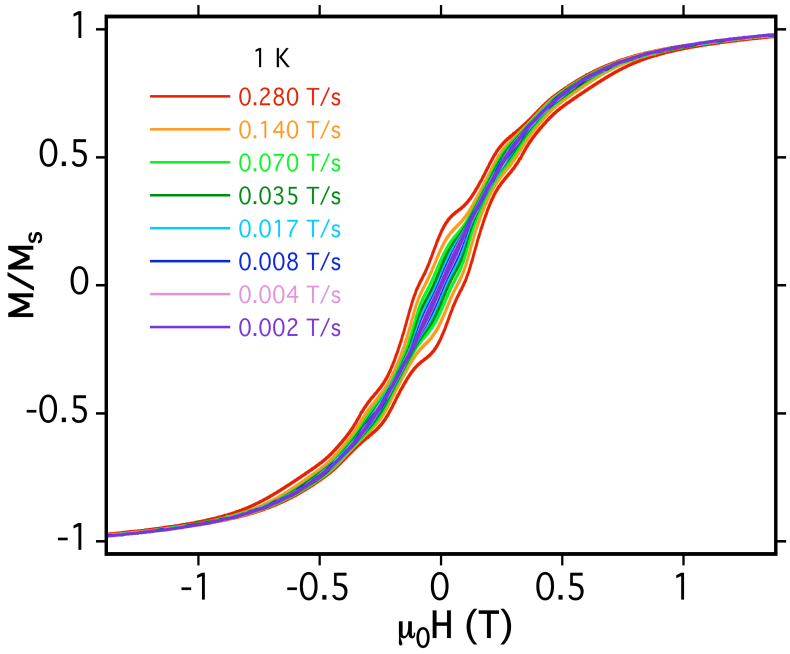


Figure S9: Magnetization (M) *vs*. applied dc field sweeps at the indicated sweep rates and at 1 K. M is normalized to the magnetization value, Ms, at 1.4 T and 40 mK .

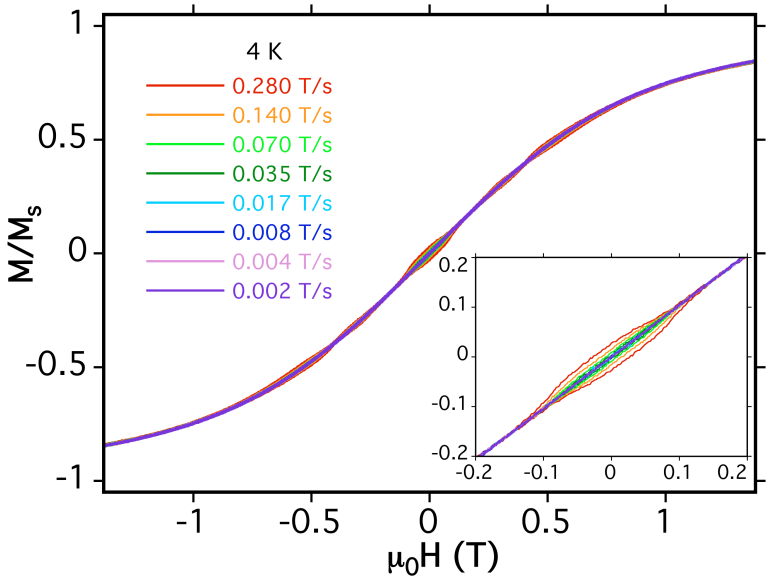


Figure S10: Magnetization (M) *vs*. applied dc field sweeps at the indicated sweep rates and at 4 K. M is normalized to the magnetization value, Ms, at 1.4 T and 40 mK. Inset: Enlargement of the central part of the hysteresis loops.

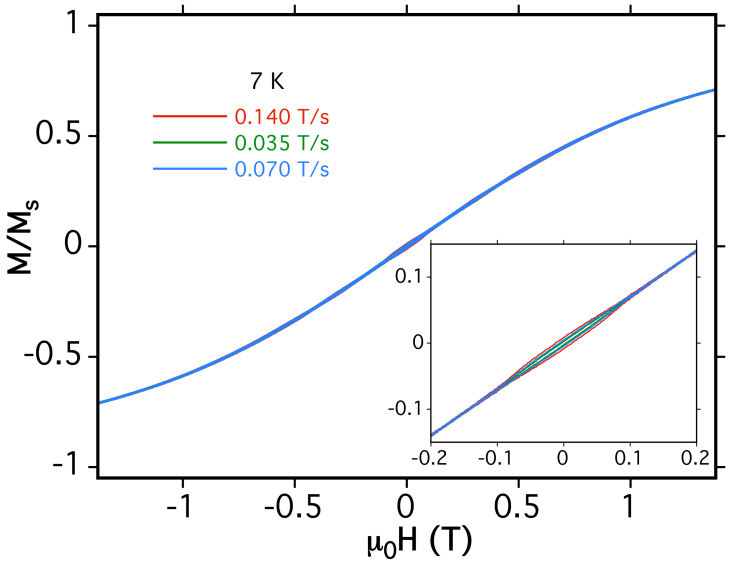


Figure S11: Magnetization (M) *vs*. applied dc field sweeps at the indicated sweep rates and at 7 K. M is normalized to the magnetization value, Ms, at 1.4 T and 40 mK. Inset: Enlargement of the central part of the hysteresis loops.

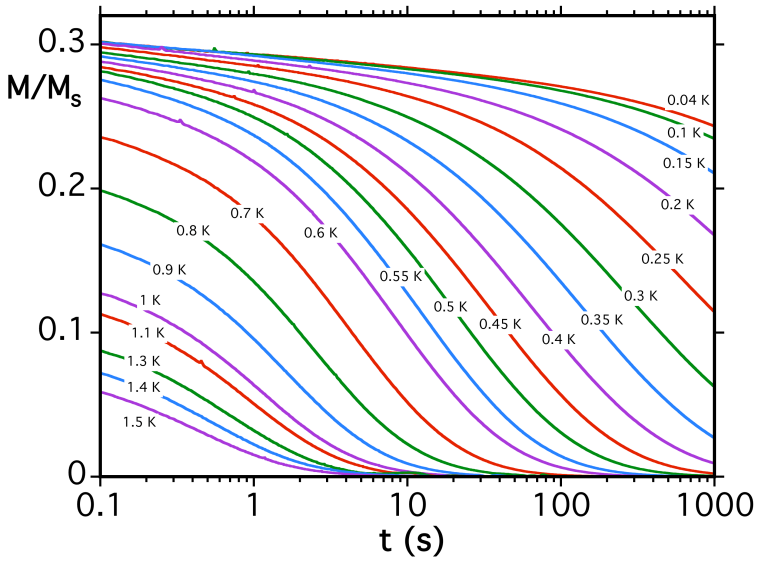


Figure S12: Relaxation decay data plotted as M/Ms *vs*. time.

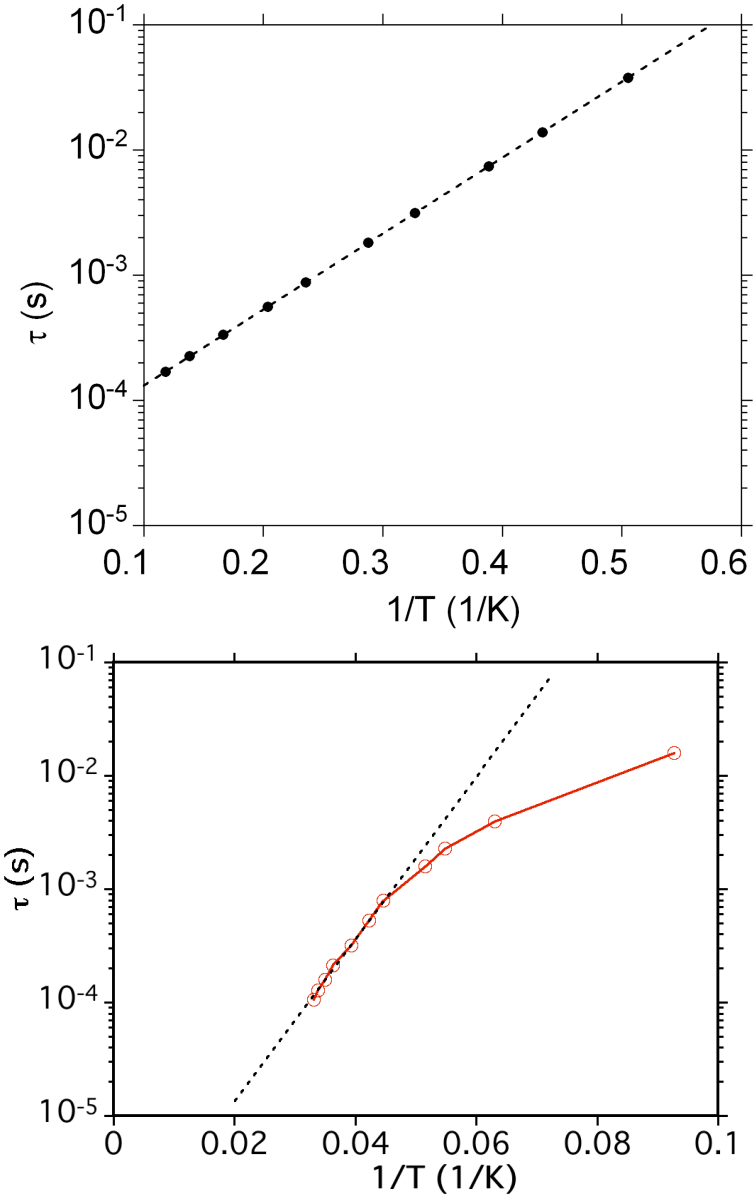


Figure S13: Arrhenius plots using ac and dc data. Top: Low temperature dynamics. Bottom: High temperature dynamics. The dashed lines are the fits of the thermally activated region, leading to the following values Top: U_{eff} = 9.7 K, τ_0 = 3.2 10^{-5} s; Bottom: U_{eff} = 170 K, τ_0 =4.10^{-7} s dynamics.