Supplementary Materials

Linking High Anisotropy Dy_3 Triangles to Create a Dy_6 Single-Molecule Magnet

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Experimental part:

Magnetism:

The magnetic susceptibility measurements were obtained with the use of a Quantum Design SQUID magnetometer MPMS-XL7 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 ground polycrystalline samples of 9.60 mg 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.

X-ray crystallography:

Crystals of $[C_{54}H_{66}Dy_6N_4O_{40}]\cdot2[NO_3]\cdot(H_2O)\cdot3(CH_3)_2CO$ were grown from acetone. A single yellow brick suitable for X-ray diffraction measurements was mounted on a glass fibre. 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 data and refinement parameters for $[C_{54}H_{66}Dy_6N_4O_{40}]\cdot2[NO_3]\cdot(H_2O)\cdot3(CH_3)_2CO$ are listed in Table 1. Interatomic distances and angles are listed in Table 3. The reflection data were consistent with a triclinic system; P-1.

The crystal structure was solved and refined using the SHELXTL program suite. The crystals were of poor quality and diffracted weakly, therefore the data were truncated at 23.26°. Direct methods yielded all non-hydrogen atoms. All hydrogen atom positions were calculated geometrically and were riding on their respective atoms. The aromatic ring C10-C15 was constrained using the command AFIX 66. The nitrate and acetone atoms were modeled with restraints (SADI, SIMU) and several were refined with isotropic thermal parameters. The acetone solvent molecules were also modeled with restraints (SADI, SIMU, FLAT) and two were refined with isotropic thermal parameters. A coordinated water molecule was disordered over two positions and was also modeled with isotropic thermal parameters. Hydrogen atoms of the water molecules could not be located from the electron density maps and are therefore included in the molecular formula but absent from the structure. Except as mentioned above, all non-hydrogen atoms were refined with anisotropic thermal parameters. The structure contains solvent accessible voids of approximately 166 Å^3, however additional electron density that could be attributed to extra solvent molecules was not observed. The largest residual electron density peak (2.263 e/Å^3) was associated with the Dy1 atom. Full-matrix least-squares refinement on F^2 gave R_1 = 0.0758 and wR_2 = 0.1703 at convergence.

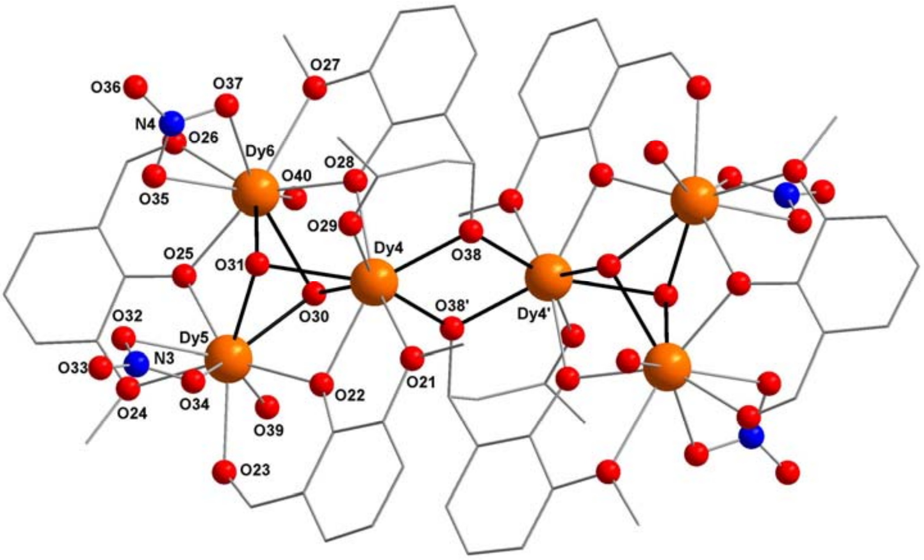


Fig. S1: The molecular structure of the second isomer of **1**.

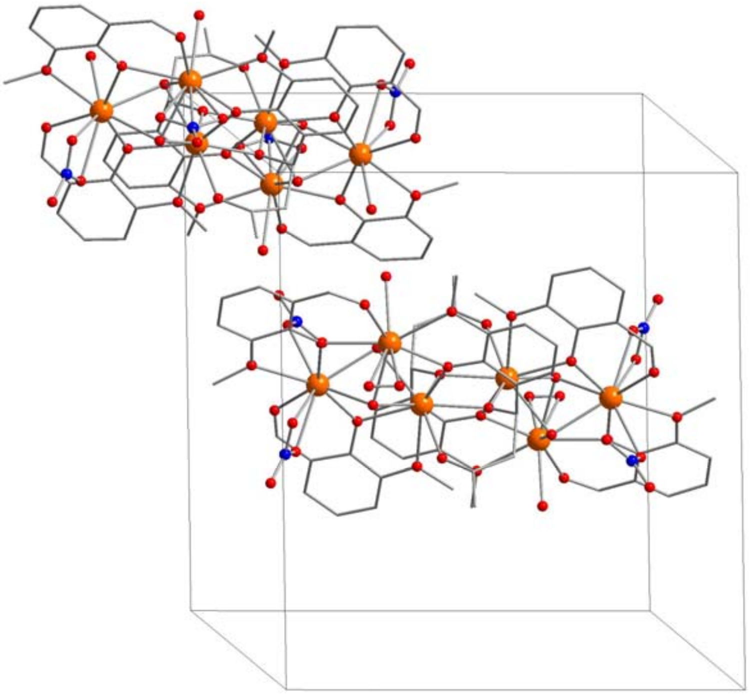


Fig. S2: Unit cell of **1** showing the relationship between the two isomers.

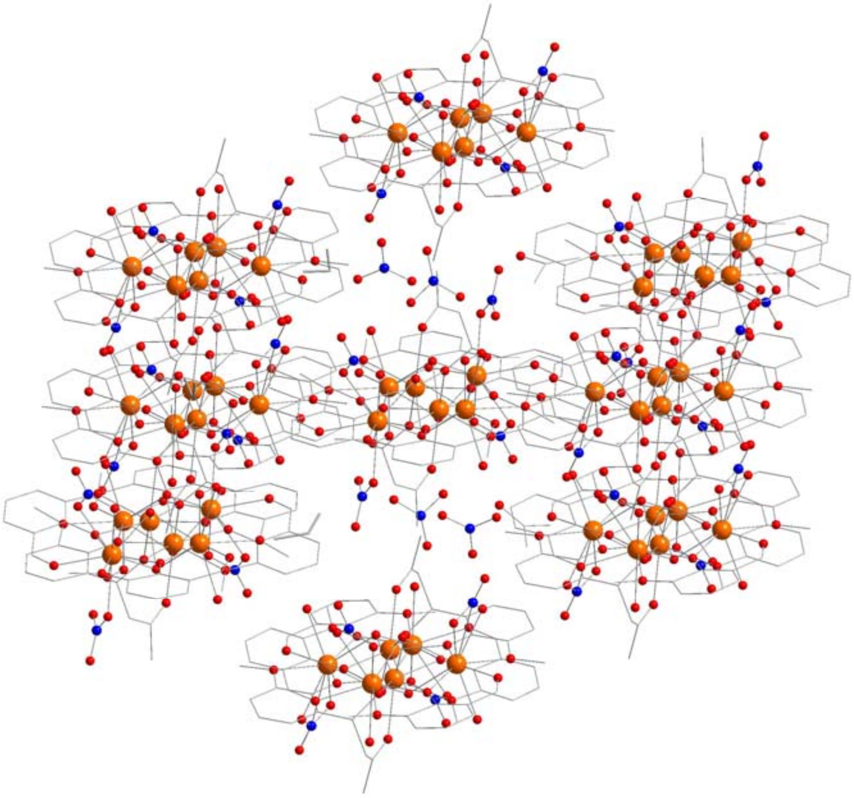


Fig. S3: Packing diagram of **1.**

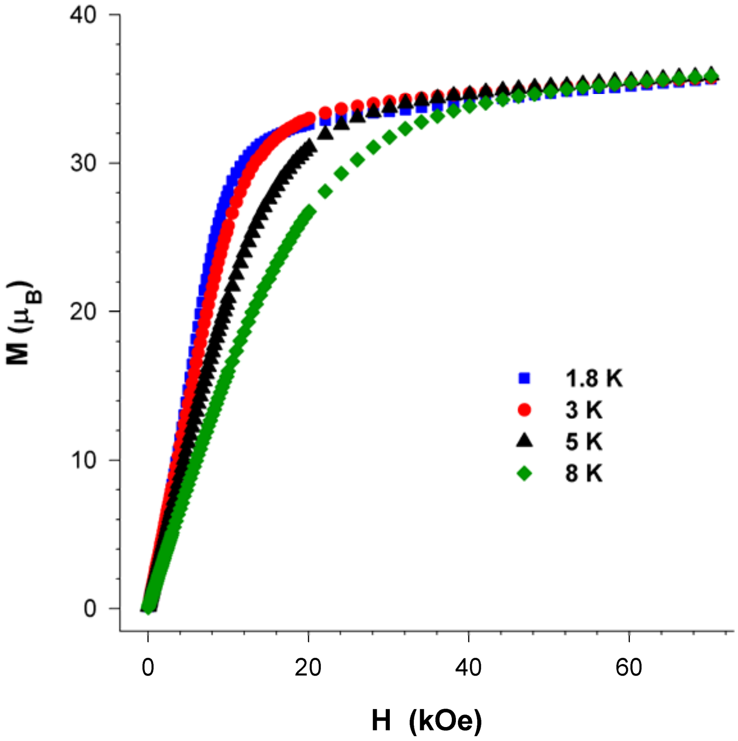


Fig. S4: Field dependence of the magnetization between 1.8 and 8 K for **1**.

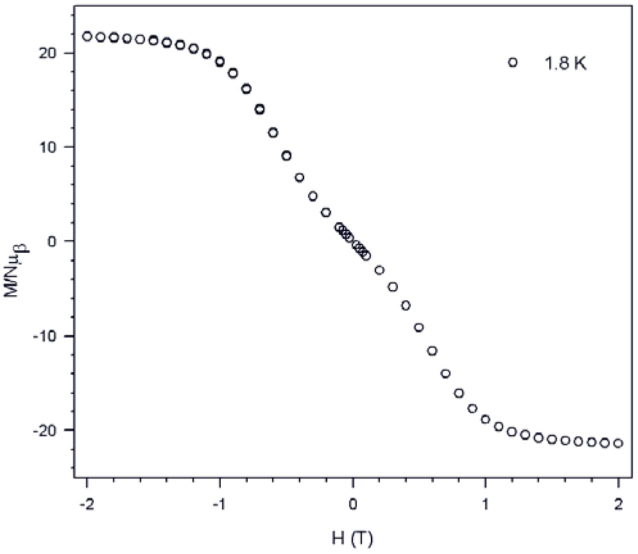
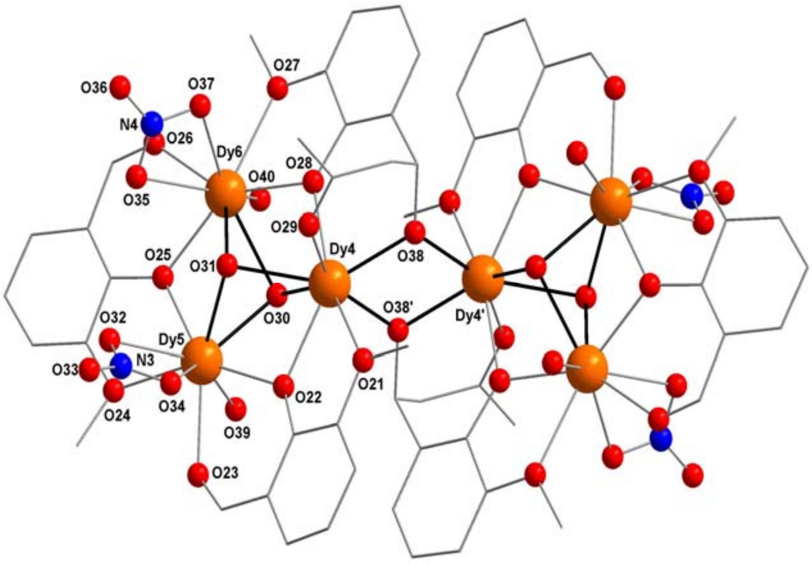


Fig. S5: Field dependence of the magnetization at 1.8 K showing the absence of hysteresis effect for **1**.



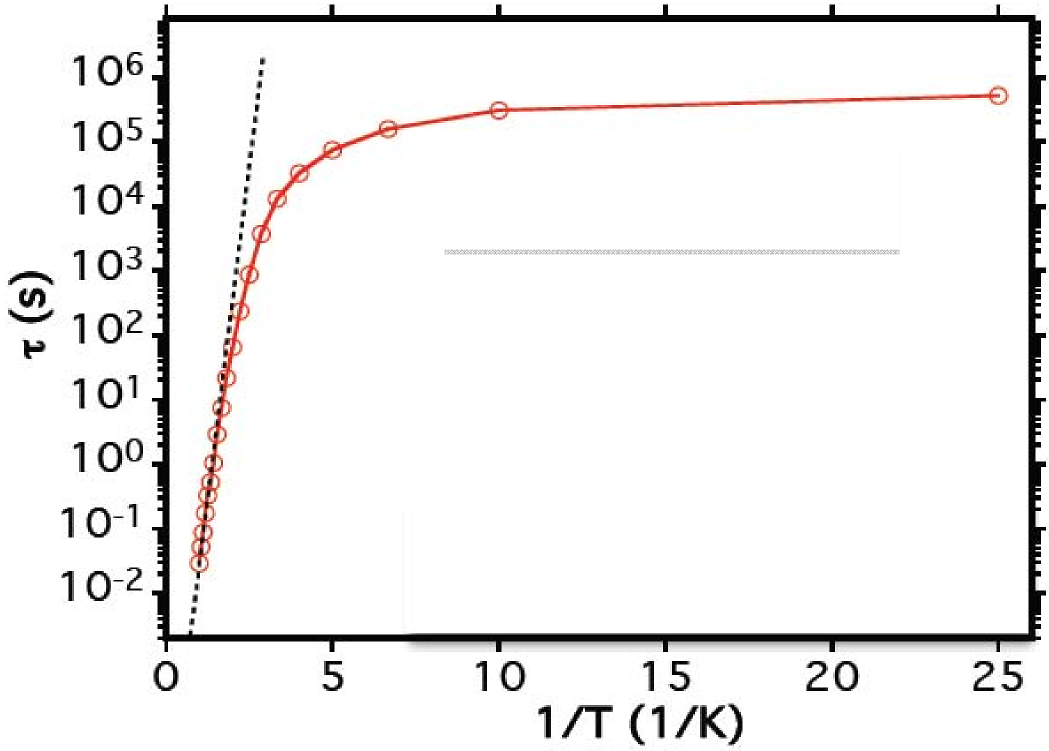


Fig. S6: Arrhenius plot for **1.**