Supplementary Information: Experimental Determination of Single Molecule Toroic Behaviour in a Dy8 Single Molecule Magnet

Qing Zhang,[a,b] Michael L. Baker,*[c,d] Shiqi Li,[a,b] Myriam P. Sarachik,*[a,b] José J. Baldoví,[e] Alejandro Gaita-Ariño[f], Eugenio Coronado[f], Dimitris I. Alexandropoulos[g] and Theocharis Stamatatos[g,h].

*a) Department of Physics, Graduate Center, CUNY, New York, New York 10016, USA & Department of Physics, City College of New York, CUNY, New York, New York 10031, USA; *E-mail: msarachik@ccny.cuny.edu*
*c) The School of Chemistry, The University of Manchester, M13 9PL Manchester, United Kingdom; *E-mail: michael.baker@manchester.ac.uk*
d) The University of Manchester at Harwell, Didcot, OX11 0FA, UK.
e) Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany.
f) Instituto de Ciencia Molecular (ICMol), Universitat de València, C/Catedrático José Beltrán, 2, E-46980 Paterna, Spain
g) Department of Chemistry, Brock University, L2S 3A1 St. Catharines, Ontario, Canada
h) Present address: Chemistry Department, University of Patras, Patras 26504, Greece

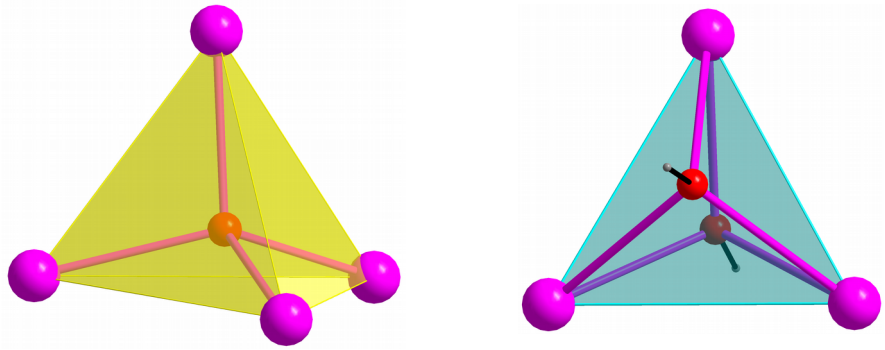

Figure. S1. Structures of the individual Dy_4 tetrahedron (left) and Dy_3 triangles (right) within the reported Dy_8 cluster. Color code as in Fig. 1.

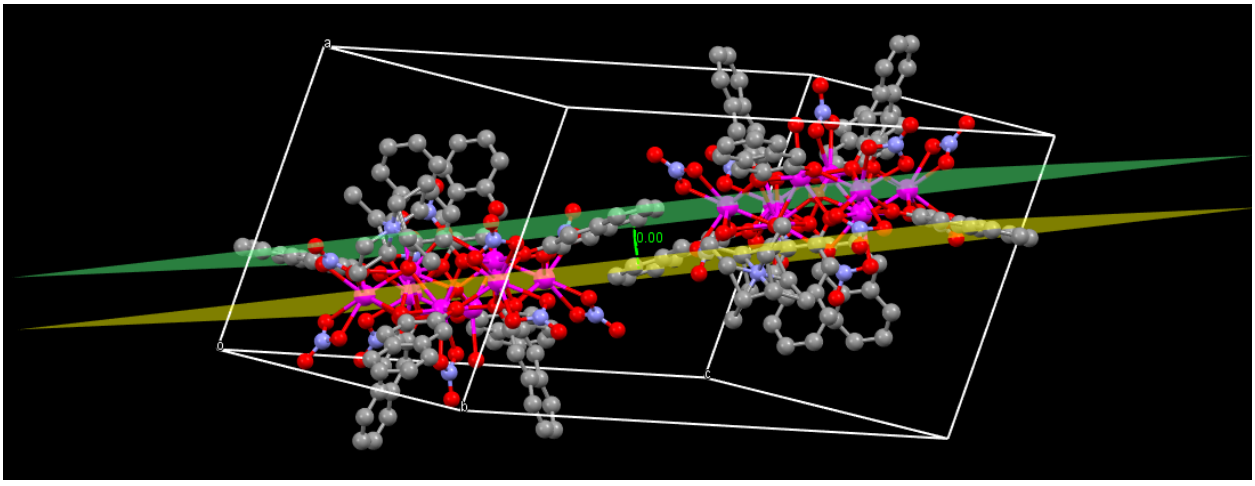

Figure S2. Enlarged Packing diagram (as shown in Fig. 1(c) of the main text) showing the orientation of the best-mean-planes between adjacent octanuclear clusters in the crystal.

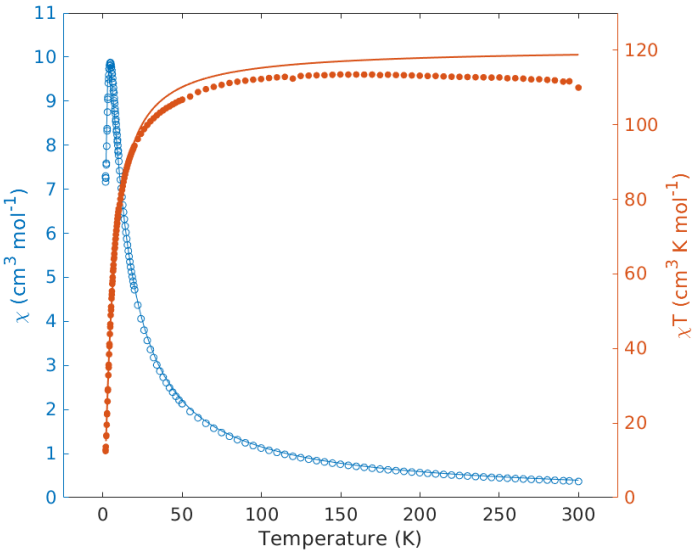

Figure S3. The temperature dependence of magnetic susceptibility (blue circles) and temperature susceptibility product (solid red circles) for a polycrystalline sample of Dy8 with an applied field of 1000 Oe. Solid line represent simulations described in the main text.

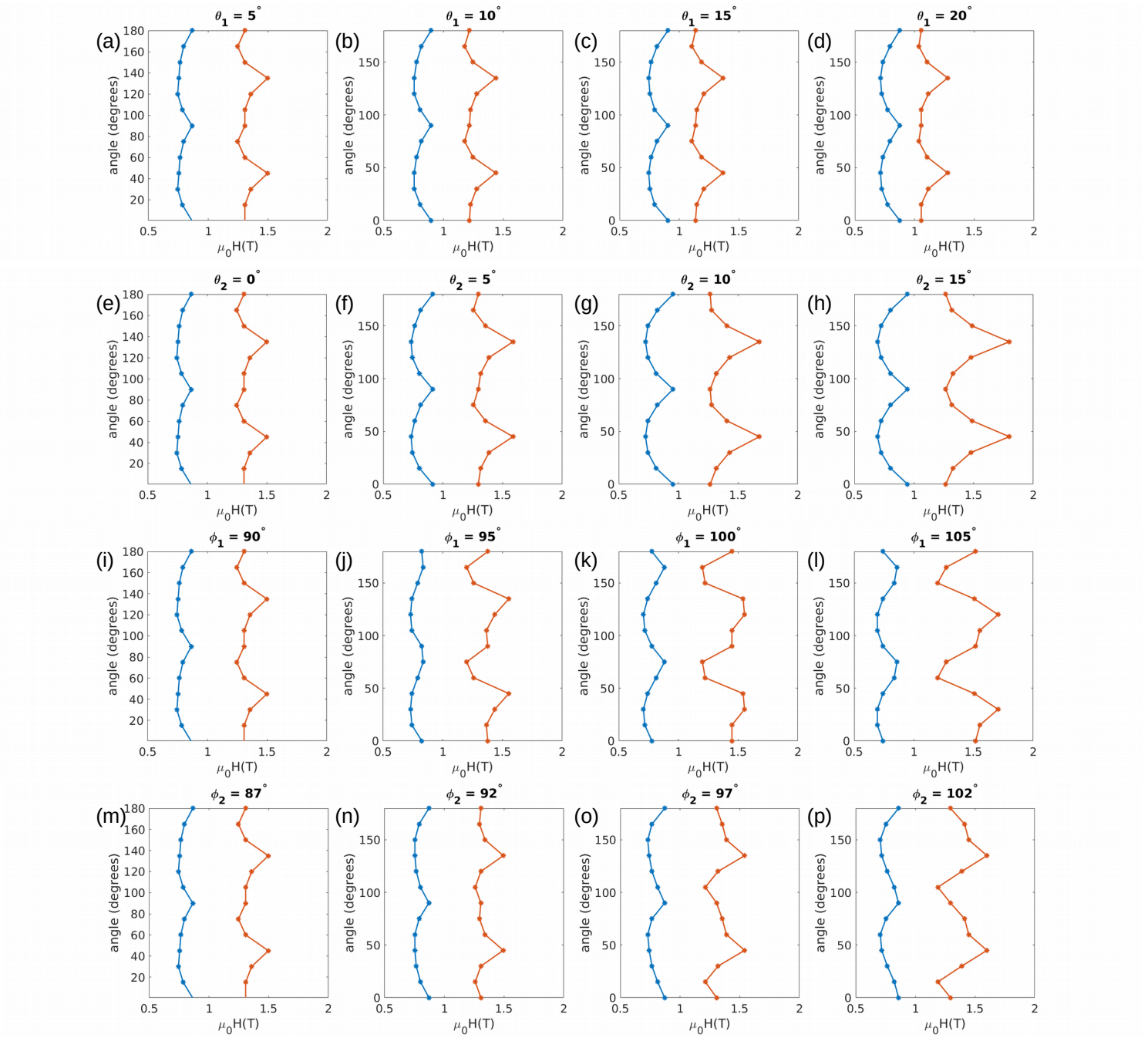

Figure S4. The results for a series of magnetisation calculations showing dM/dH maxima for a series of Dy8 models with different Dy ion easy axis orientations. The blue points represent the maximum in dM/dH due to field induced crossing c_1. The red points represent maxima in dM/dH due to field induced crossing c_2. Running from left to right, the single ion easy axis directions are adjusted from the best fit values. Panels (a), (e), (i) and (m) show the best fit result. The top row (a to d) show the effect of adjusting θ_1 from the best fit value ($\theta_1 = 5°$) . The second row (e to h) show the effect of adjusting θ_2 from the best fit value ($\theta_2 = 0°$). The third row (i to l) show the effect of adjusting Φ_1 from the best fit value ($\Phi_1 = 90°$). The forth row (m to p) show the effect of adjusting Φ_2 from the best fit value ($\Phi_2 = 87°$).

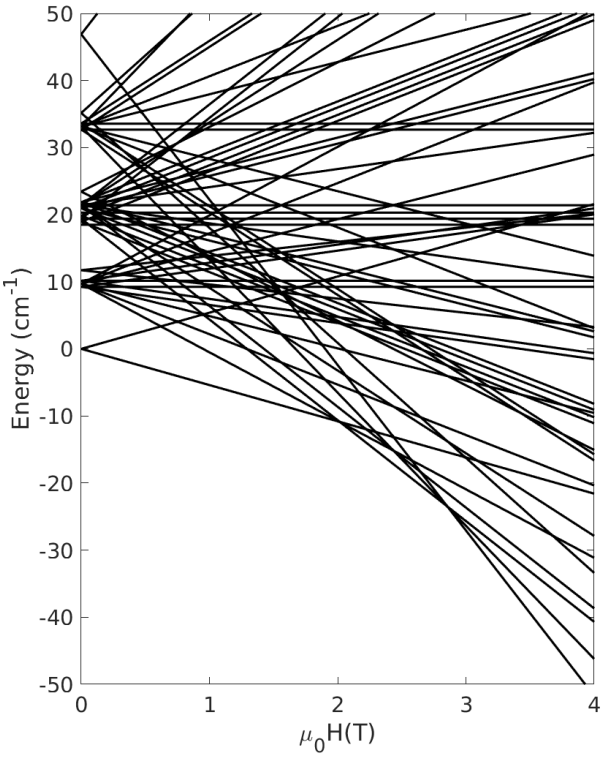

Figure S5. Zeeman energy diagram for out of plane magnetisation (magnetic field applied along the molecular Z axis, defined within the main text). Ground state crossings are obtained at 2 and 2.84 T in addition to several low energy excited state crossings.