

ELECTRONIC SUPPLEMENTARY INFORMATION

to

A decanuclear $[\text{Dy}^{\text{III}}_6\text{Zn}^{\text{II}}_4]$ cluster: a $\{\text{Zn}^{\text{II}}_4\}$ rectangle surrounding an octahedral $\{\text{Dy}^{\text{III}}_6\}$ single molecule magnet †

Nikoleta Stavgianoudaki,^a Milosz Siczek,^b Tadeusz Lis,^b Giulia Lorusso,^c Marco Evangelisti^c and Constantinos J. Milios*^a

^a Department Of Chemistry, University of Crete, Voutes 71003, Herakleion, Greece. Fax: +30-2810-545001; Tel: +30-2810-545099; E-mail: komil@uoc.gr

^c Faculty of Chemistry, University of Wrocław, Joliot-Curie 14, Wrocław 50-383, Poland.

^d Instituto de Ciencia de Materiales de Aragón (ICMA), CSIC – Universidad de Zaragoza, 50009 Zaragoza, Spain

Materials and physical measurements

All manipulations were performed under aerobic conditions, using materials as received. Elemental analyses (C, H, N) were performed by the University of Ioannina microanalysis service. Variable-temperature, solid-state direct current (dc) magnetic susceptibility data down to 2.0 K were collected on a Quantum Design MPMS-XL SQUID magnetometer equipped with a 5 T DC magnet at the University of Zaragoza. Diamagnetic corrections were applied to the observed paramagnetic susceptibilities using Pascal's constants. Powder XRD measurements were collected at room temperature on a freshly prepared sample of **1** on a PANalytical X'Pert Pro MPD diffractometer at the University of Crete.

Synthesis

Zn(OAc)₂·2H₂O (1 mmol, 0.220 g), Dy(NO₃)₃·5H₂O (1 mmol, 0.440 g) and H₃L (1 mmol, 0.297 g) were added in MeOH (15 ml) in presence of base NEt₃ (1 mmol, 0.140 ml) and the resulting mixture was transferred to a Teflon-line autoclave (23 ml) and kept at 95 °C for 12 hours. After slow cooling to room temperature at a rate of 20 °Ch⁻¹ pale yellow crystals of [Dy₆Zn₄O₂(L)₂(HL)₂(OAc)₈(CH₃O)₄(H₂O)₂]·4MeOH (**1**·4MeOH) were obtained in good yield (~35%) and collected by filtration, washed with Et₂O and dried in air. Elemental Anal. calcd (found) for **1**·2MeOH: C 32.67 (32.54), H 3.52 (3.69), N 1.88 (1.77)%.

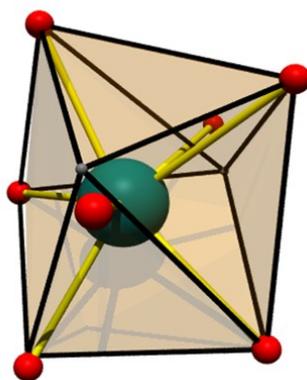


Figure S1. Capped trigonal prismatic geometry for Dy1 in complex **1** as calculated with SHAPE.

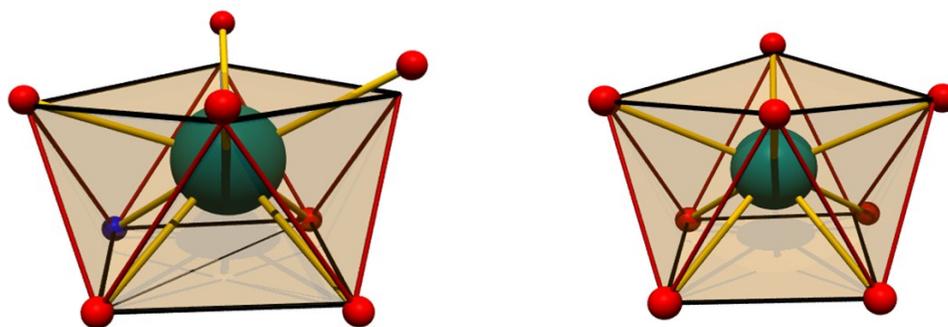


Figure S2. Square antiprismatic geometry for Dy₂ (left) and Dy₃ (right) in complex **1** as calculated with SHAPE.

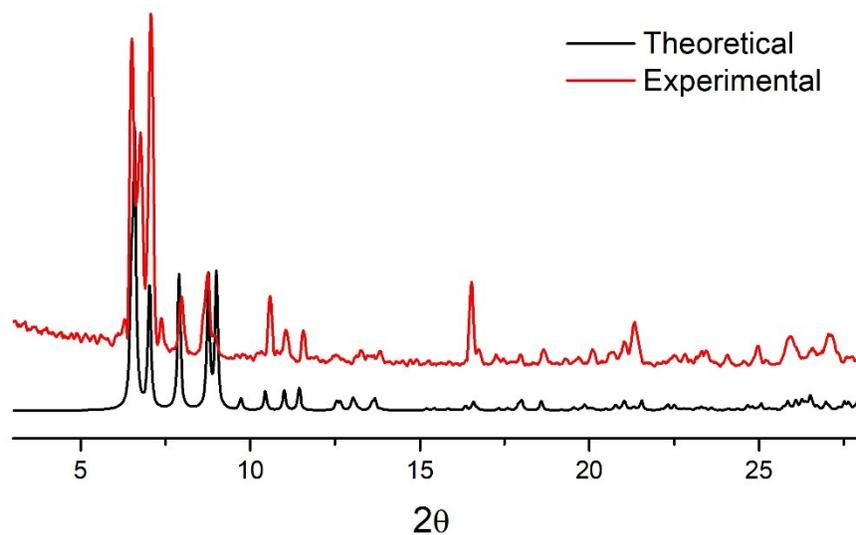


Figure S3. Powder XRD diagrams' comparison between **1** and its simulated pXRD diagram. The difference in the peaks' intensity is probably due to partial decomposition of the crystals caused by loosing of methanol of solvation.

