Electronic Supplementary Information (ESI)

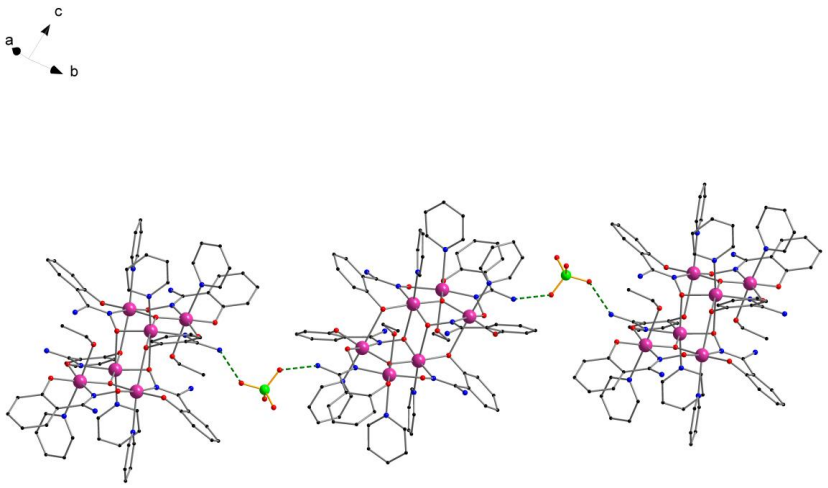
A cationic and ferromagnetic hexametallic Mn(III) Single-Molecule Magnet based on the salicylamidoxime ligand

José Martínez-Lillo,* Neil Dolan and Euan K. Brechin*

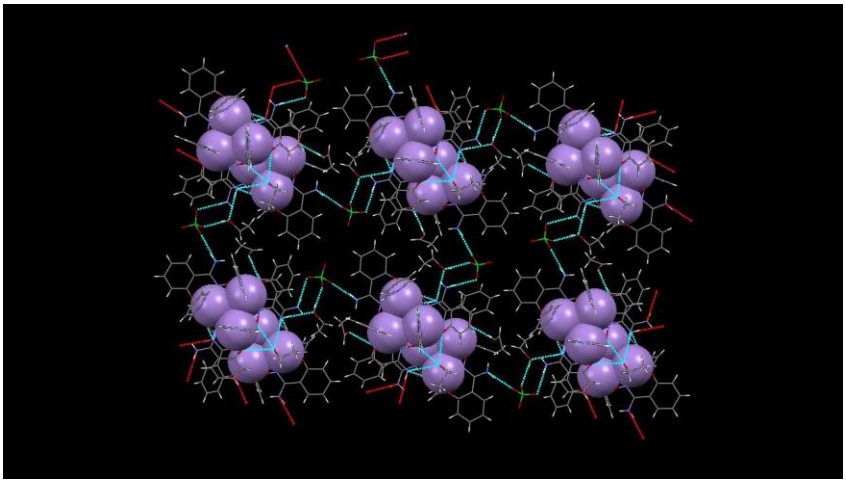
EaStCHEM School of Chemistry, The University of Edinburgh, West Mains Road, EH9 3JJ, Edinburgh, Scotland, UK. E-mails: fmartine@staffmail.ed.ac.uk and ebrechin@staffmail.ed.ac.uk. Tel: +44 (0)131 650 7545. Fax: +44 (0)131 650 6453.

Preparation of 1. All manipulations were performed under aerobic conditions, using materials and solvents as received. $Mn(ClO_4)_2 \cdot 6H_2O$ (0.249 g, 6.88 mmol) was dissolved with continuous stirring in EtOH (20 mL), then H_2N-saoH_2 (0.102g, 6.70 mmol) was added followed by pyridine (1mL, 12.4 mmol) and NEt_3 (0.05 mL, 3.58 mmol). The dark green final solution was left to evaporate in a fumehood at room temperature. Dark green crystals were formed in 1 day, which were suitable for X-ray diffraction studies. Yield: 72%. Anal. Cald. (found) for $C_{76}H_{78}O_{24}N_{18}Cl_2Mn_6$ (**1**): C, 45.0 (45.5); H, 3.9 (4.1); N, 12.4 (12.3) %. IR peaks (ATR/cm^{-1}): 1597, 1086, 1036, 1017, 878, 700, 673, 638, 628.

A)



B)



C)

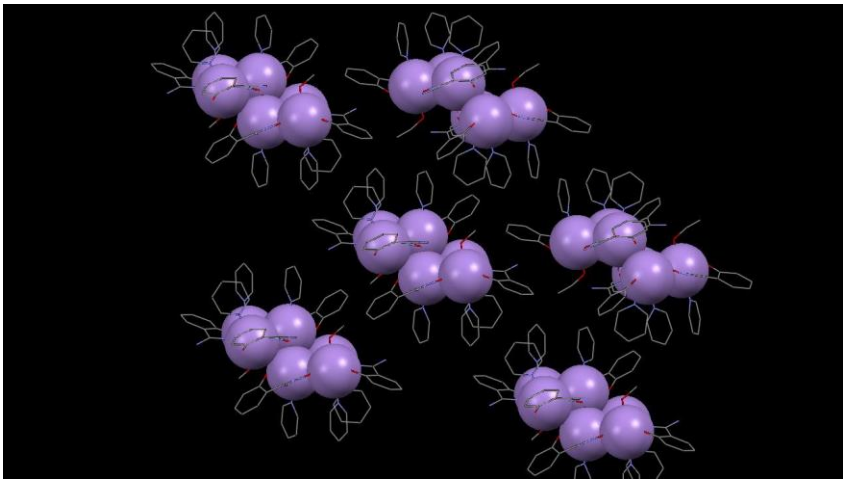


Figure S1. (**A**) Perspective view of the unidimensional arrangement of $[Mn_6(\mu_3\text{-}O)_2(H_2N\text{-}sao)_6(py)_6(EtOH)_2]^{2+}$ cations and ClO_4^- anions in **1** through H-bonding interactions (dashed lines). Solvent molecules have been omitted for clarity. [Colour code: pink, Mn; red, O; blue, N; black, C; green, Cl]. (**B**) Expansion of this interaction into 2 dimensions, highlighting the H-bonded square sheets. (**C**) View of the interdigitated Mn_6 cluster cations in the third dimension.

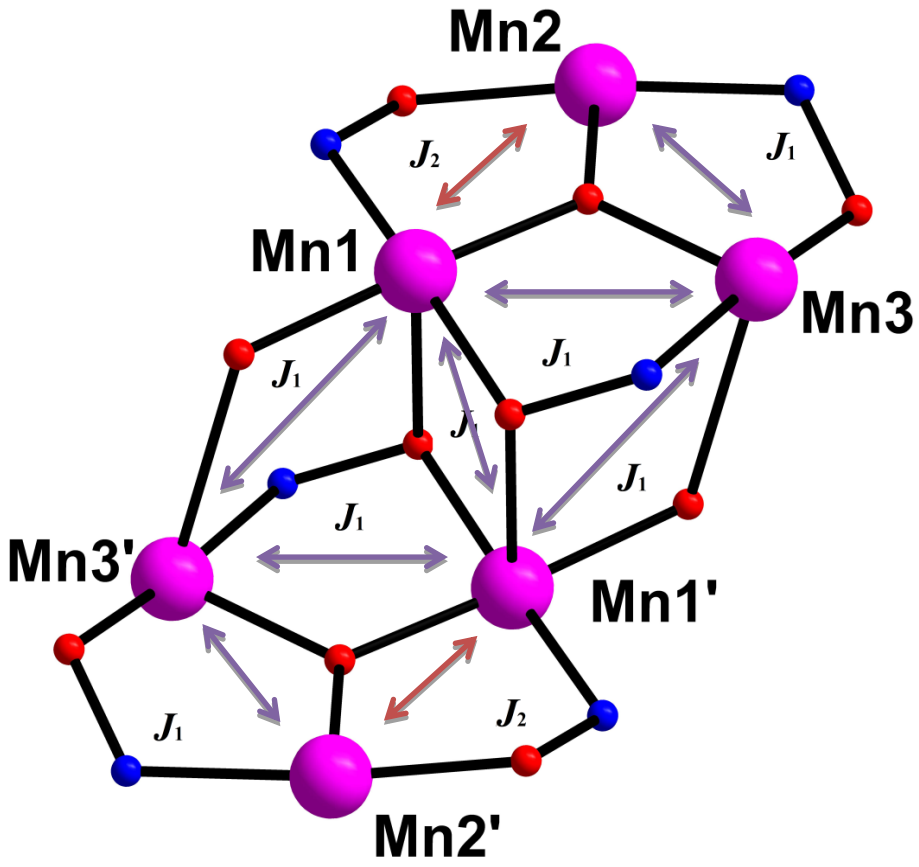


Figure S2. Two *J* coupling exchange model used for the fit of compound **1**.

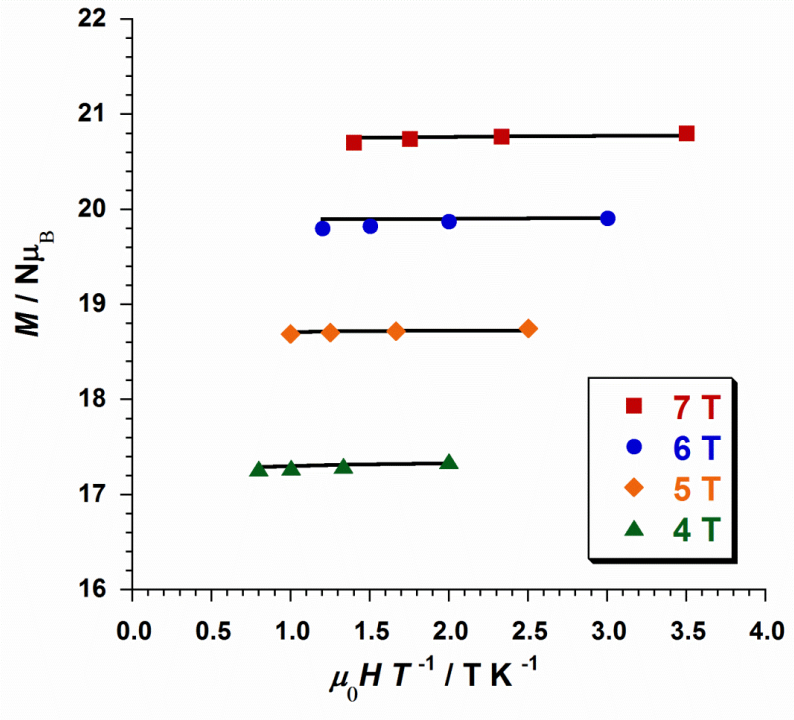


Figure S3. Plot of the reduced magnetisation ($M/N\mu_B$ *vs.* H/T) for **1** in 4, 5, 6 and 7 T fields and temperatures 2–7 K. The solid lines represent the best fit of the experimental data with $S = 12$, $g = 1.98 \pm 0.02$ and $D_{cluster} = -0.34 \pm 0.02$ cm^{-1}.