Supplementary Material (ESI) for Journal of Materials Chemistry

Supplementary Information; Paper B602858F
L. F. Jones et al. J. Mater. Chem Special Issue Eds Coronado, Gatteschi
Data for Deposition; Figs S1 to S7; Structure of 3; Magnetism of 1 and 2, EPR of 2

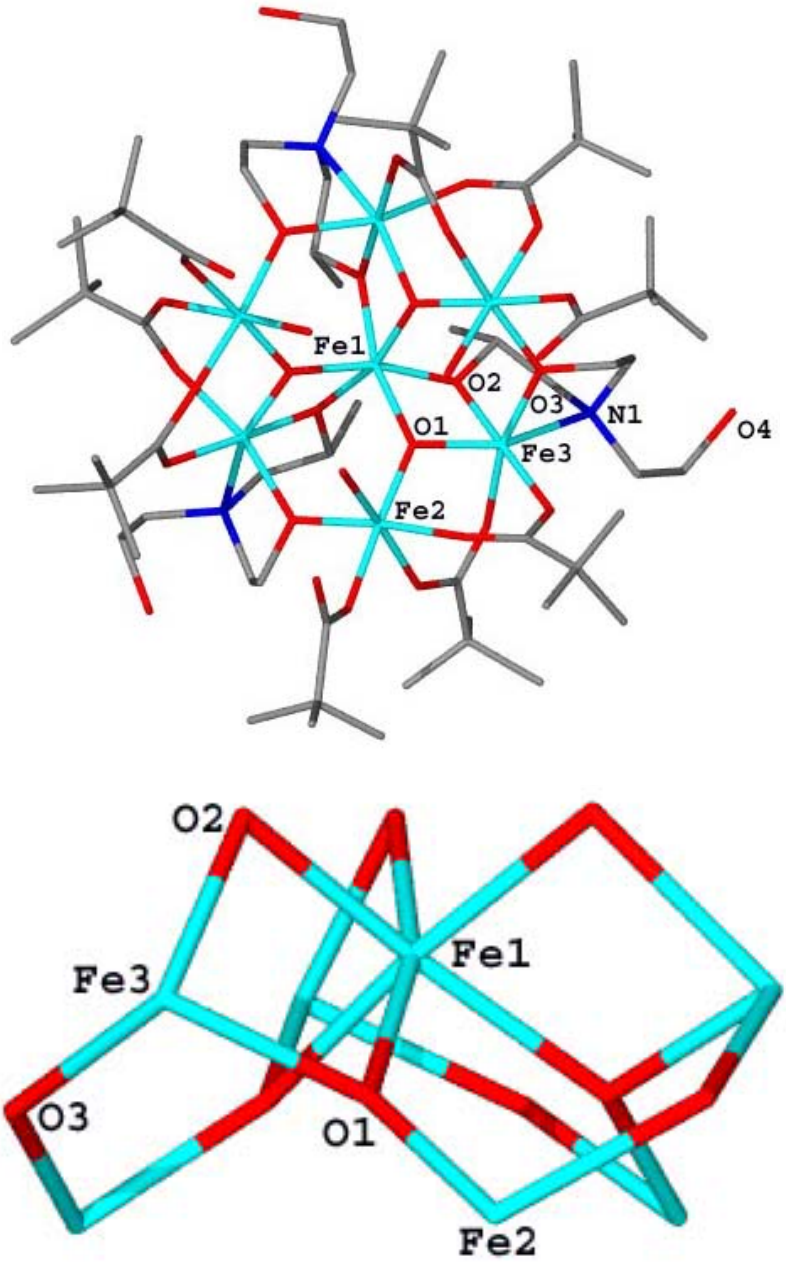

Fig. S1 (bottom) Structure of the dome-like core in **3** (top) Structure of the heptanuclear cluster **3**, H atoms omitted for clarity

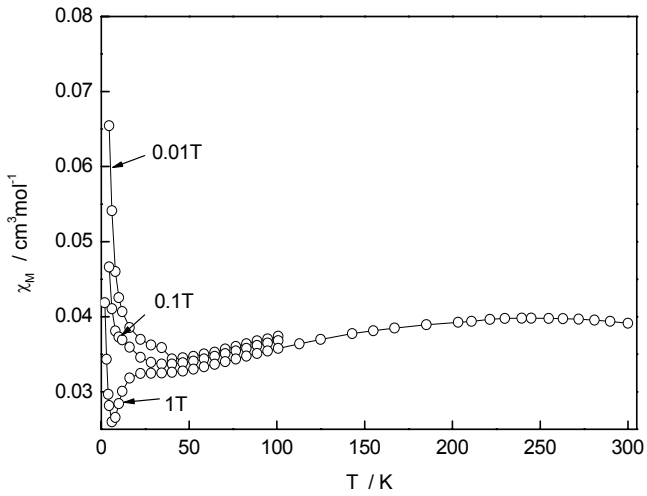

Fig S2 Plots of χ_M, per Fe_6, for $[Fe^{III}_8O_3(O_2CCH_2CH_3)_6(tea)(teaH)_3(F)_3].MeOH.H_2O$ (**1**) in fields of 1T (2 – 300 K) and 0.1 and 0.01 T (2 – 100 K)

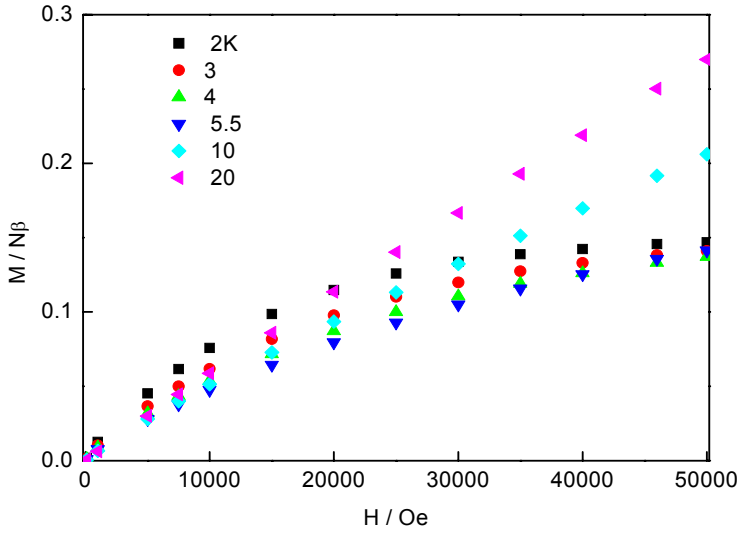

Fig S3 Magnetisation isotherms for compound $[Fe^{III}_8O_3(O_2CCH_2CH_3)_6(tea)(teaH)_3(F)_3].MeOH.H_2O$ (**1**)

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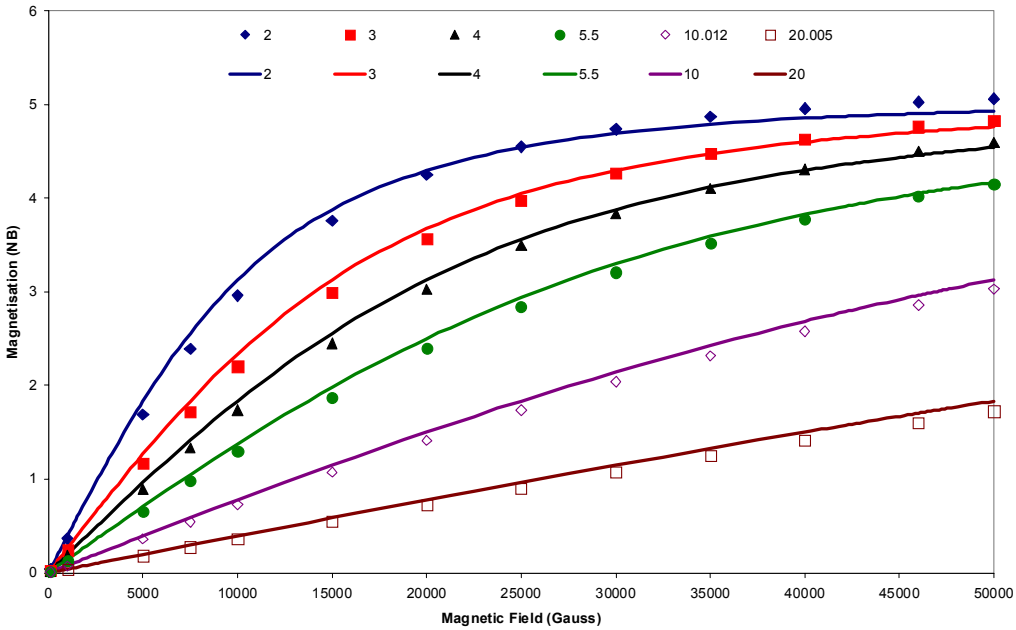

Fig S4 Magnetisation isotherms for $[Fe^{III}_7O_3(O_2CCMe_3)_9(bheapH)_3(H_2O)_3]$ (**2**), with solid lines calculated using a $S = 5/2$ Brillouin function and $g = 2.0$

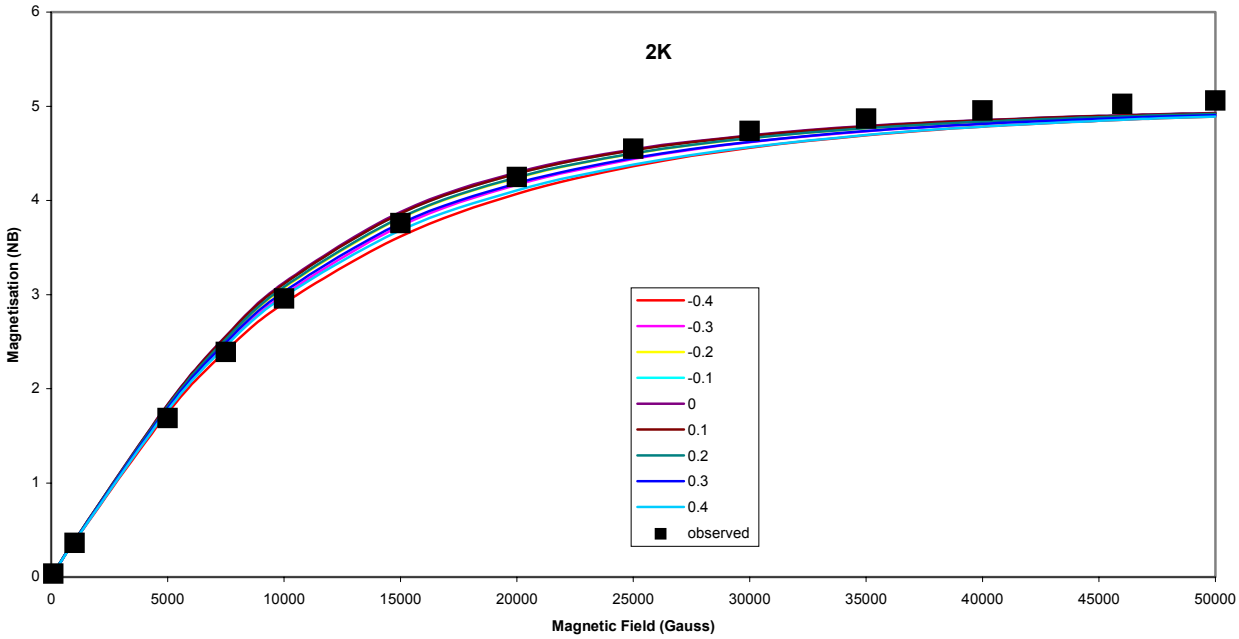

Fig S5 Magnetisation isotherm values for **2** shown as solid squares, at 2 K, and calculated values plotted for D varying between +/- 0.4 cm^{-1} using an axial $D\mathbf{S}_z^2$ spin Hamiltonian. (see colour codes in inset)

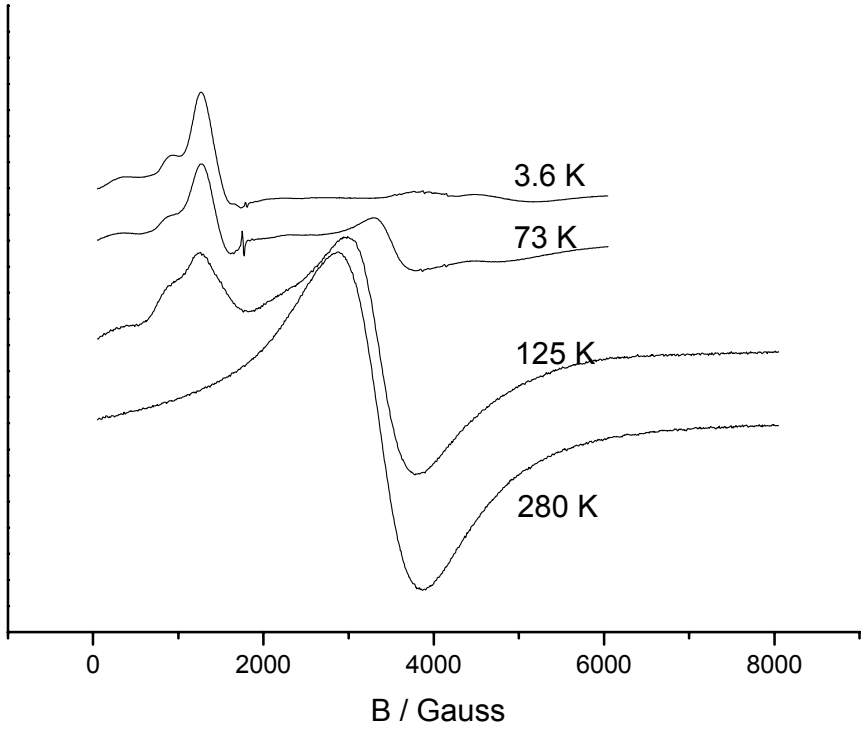

Fig S6 EPR spectra of polycrystalline powders of (compound **2**) at the indicated temperatures. Microwave frequency for 280 K and 125 K was 9.433 GHz, for 72 K and 3.6 K, 9.700 GHz. Microwave power 1.05 mW, field scan time 83.886 s, time constant 20 ms. relative spectral intensities arbitrarily scaled.

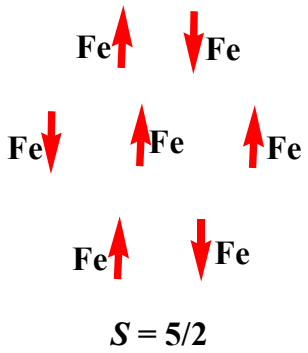

Fig. S7 Model for the $S = 5/2$ ground spin rationale in **2** and **3**