Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information for:

Acetate-Controlled Demetalation in Multiiron Polyoxometalates: A Triiron Cluster Trapped Between β- and γ-Keggin Isomers

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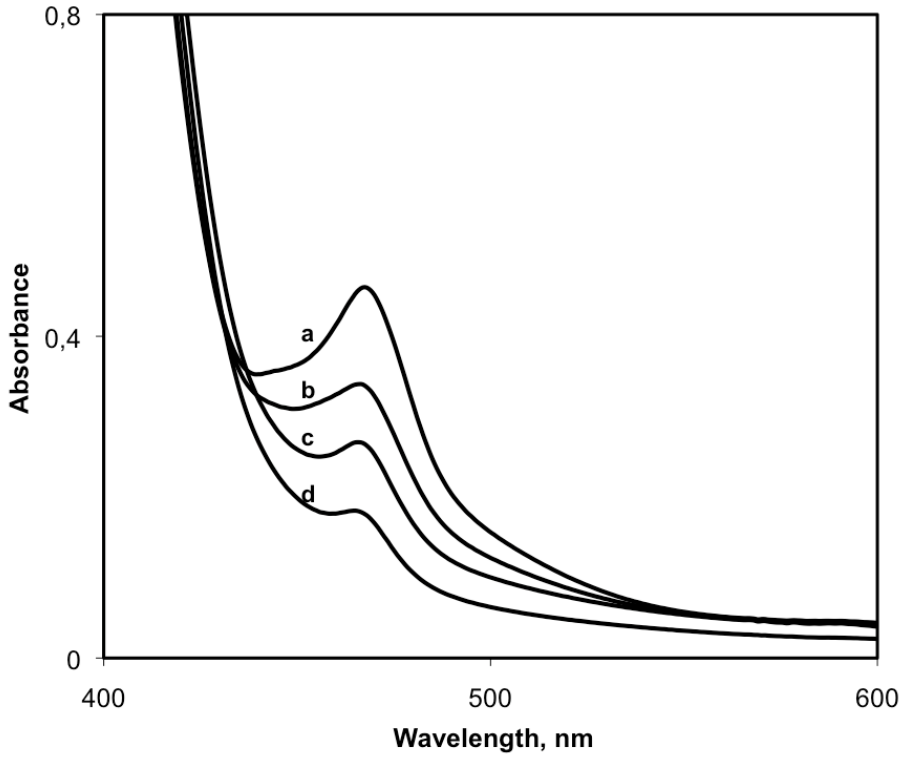

Fig. S1. Time dependence of the electronic absorption spectrum of a 40 mM aqueous solution (1 mm cell path length) of $K_{10}[(CH_3)_2(NH_2)]_2$**4**$\cdot 20H_2O$: (a) fresh solution; and after: (b) 2 hours; (c) 24 hours; (d) 6 days.

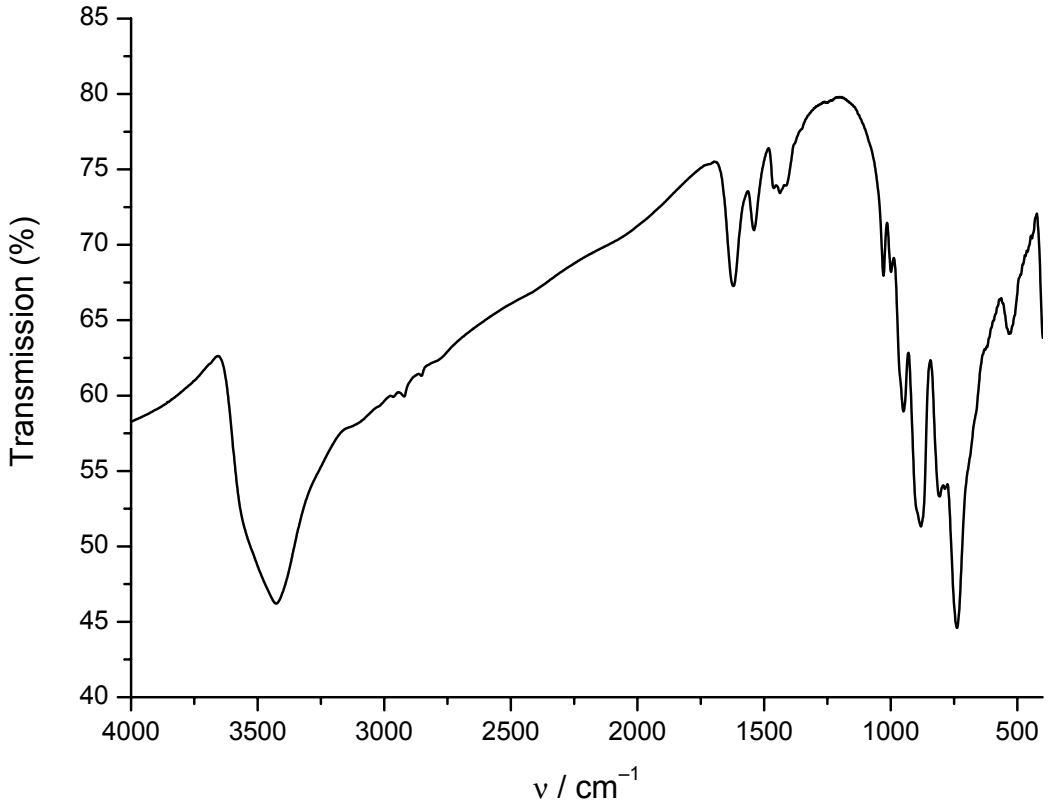

Fig. S2. FT-IR (KBr pellet) spectrum of $K_{10}[(CH_3)_2(NH_2)]_2$**4**$\cdot 20H_2O$.

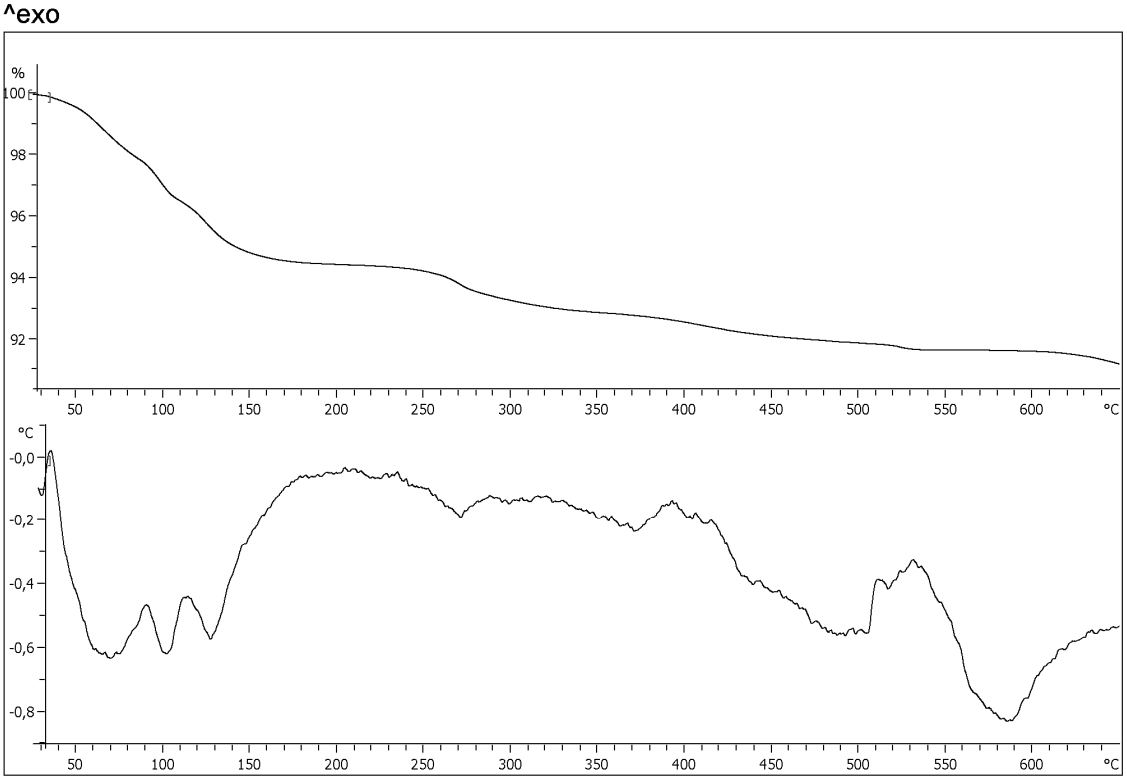

Fig. S3. TGA (top) and DTA (bottom) data of $K_{10}[(CH_3)_2(NH_2)]_2$**4**$\cdot 20H_2O$ (heating rate: 5 °C/min, N_2 atmosphere with a 60 ml/min flow rate). Note that the first mass loss of 5.5% up to 200 °C corresponds to the loss 20 crystal water molecules.

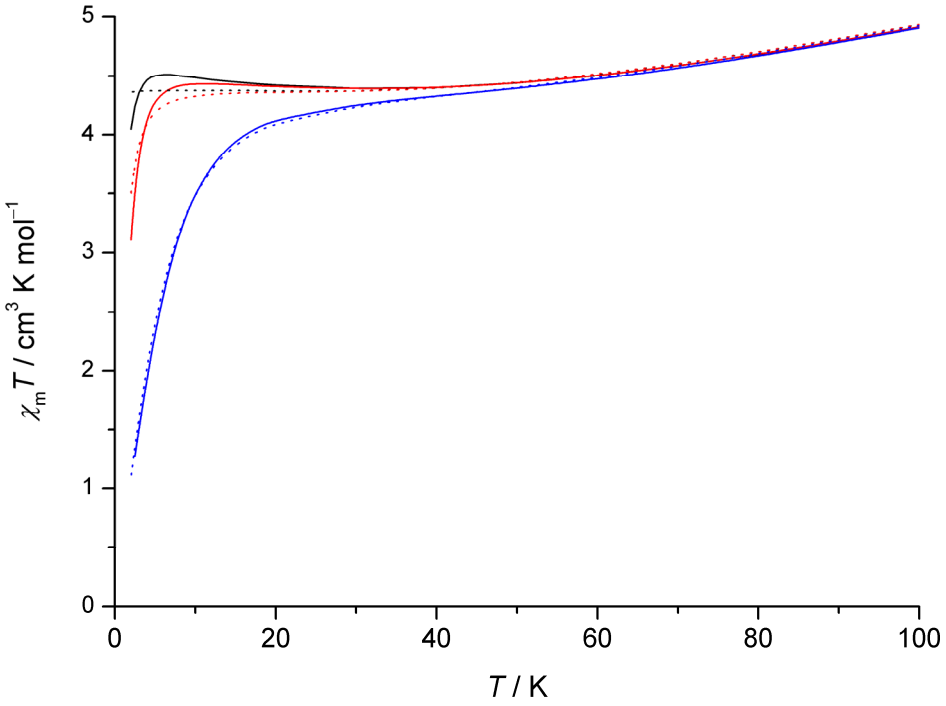

Fig. S4. Comparison of the simulated susceptibility data for $K_{10}[(CH_3)_2(NH_2)]_2$**4**$\cdot 20H_2O$ for the temperature interval 2 – 100 K. Solid lines represent least-squares fits to the experimental susceptibility for 0.1 (black), 1.0 (red) and 5.0 Tesla (blue) for the full model described in the text. Dotted curves represent the corresponding simulated curves for a pure spin Heisenberg system (without ligand field contributions).

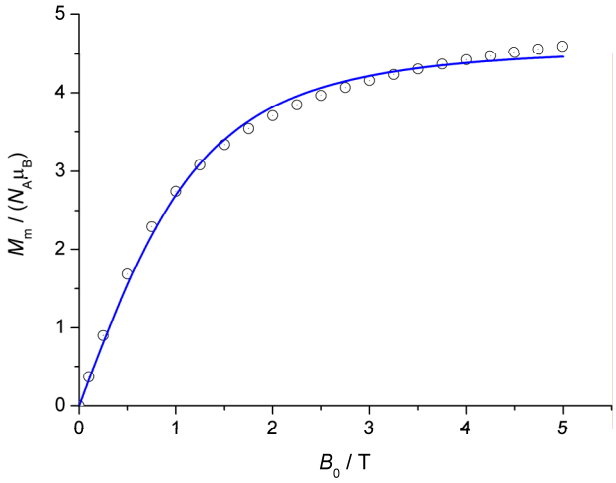

Fig. S5. Field-dependent magnetization measurements of $K_{10}[(CH_3)_2(NH_2)]_2$**4**$\cdot 20H_2O$ at 2.0 K and best least-squares fit to Brillouin function.