SUPPORTING INFORMATION

3-D Ferromagnetic Network of Mn_{12} Single-Molecule Magnets: Subtle Environmental Effects and Switching to Antiferromagnetic

Adeline Fournet,[†] Kylie J. Mitchell,[†] Wolfgang Wernsdorfer,[‡] Khalil A. Abboud,[†] and George Christou*,[†]

[†] Department of Chemistry, University of Florida, Gainesville, FL 32611, USA. [‡] Institut Néel-CNRS and University Grenoble Alpes, F-38000 Grenoble, Cedex 9, France.

* Corresponding author: christou@chem.ufl.edu

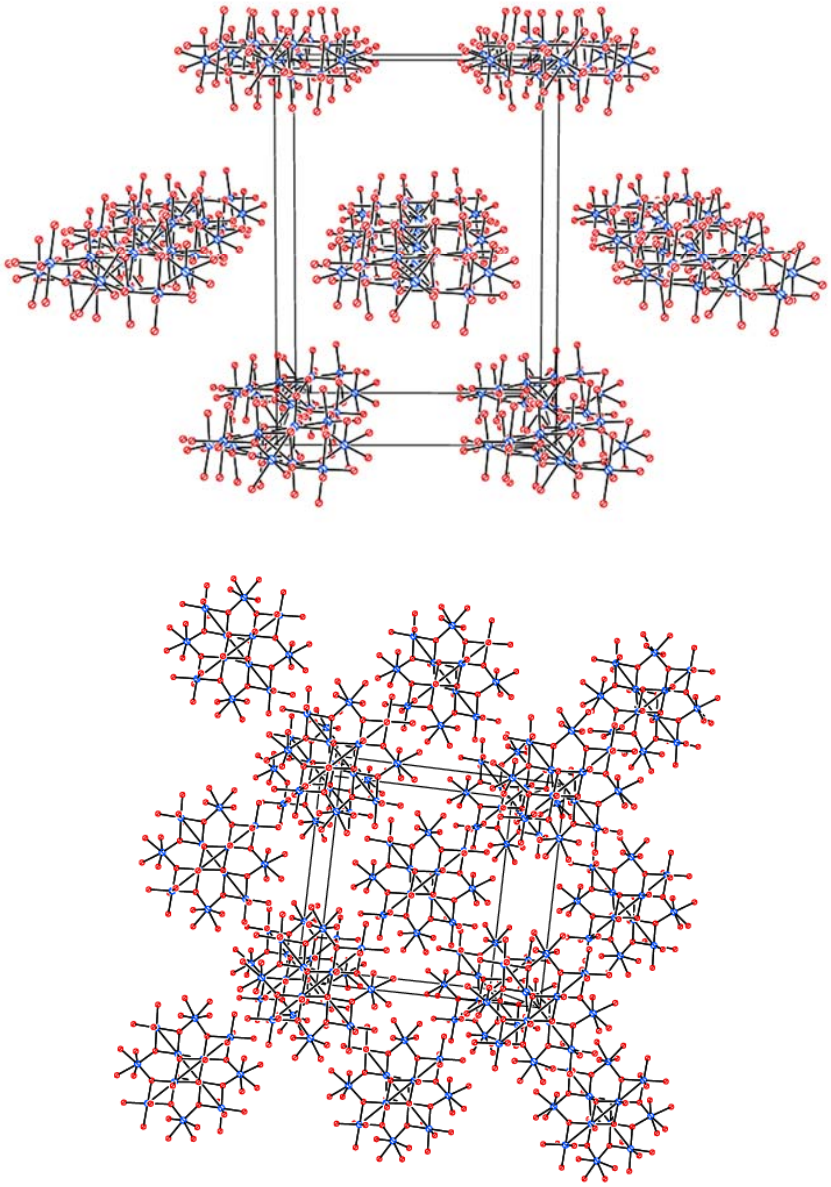

Figure S1. Side- and top-view of the body-centered cubic packing of complex **2**·8MeCN emphasizing the identical orientation of molecules and collinear z-axes. For clarity, only Mn and O atoms are shown.

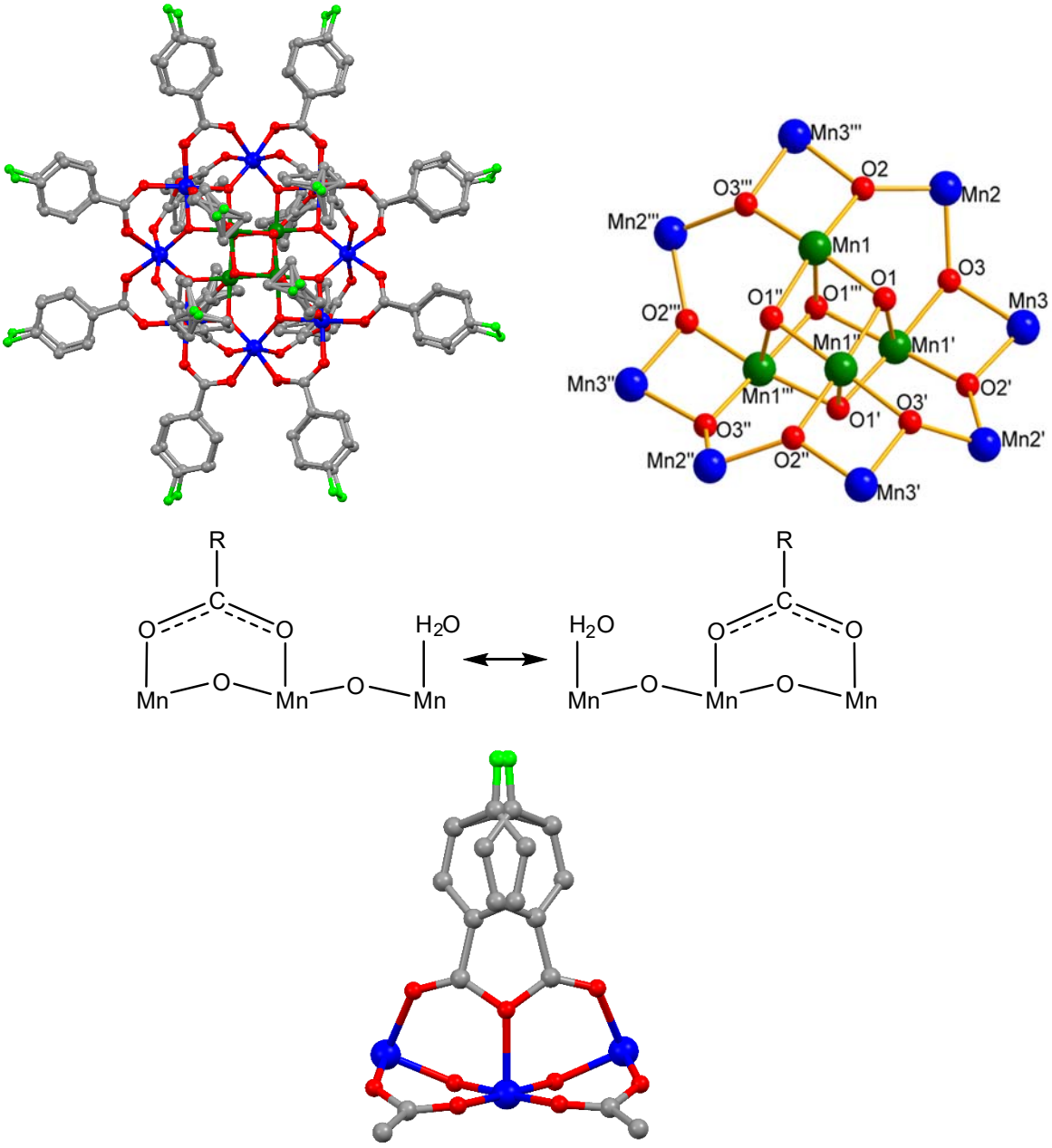

Figure S2. (top) Complete molecule emphasizing disorder of all carboxylates (left) and {$Mn_{12}O_{12}$} core showing atom labeling. (middle) Carboxylate/water disorder caused by the crystallographic mirror plane, and (bottom) the resulting appearance at this position. Color code: Mn^{III} blue, Mn^{IV} green, O red.

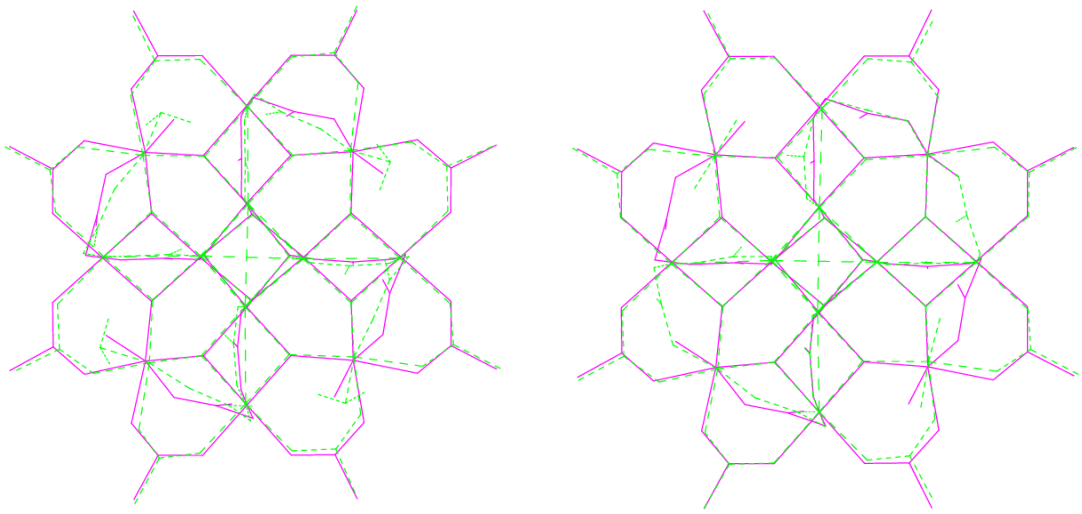

Figure S3. Overlay of the core of complex **2** (purple) with (left) the core of complex **1** (green), and (right) the core of $[Mn_{12}O_{12}(PhCO_2)_{16}(H_2O)_4]$ (**3**) (green). The carboxylate O atoms and first two C atoms are shown for clarity but were not included in the RMS calculations of Table S1.

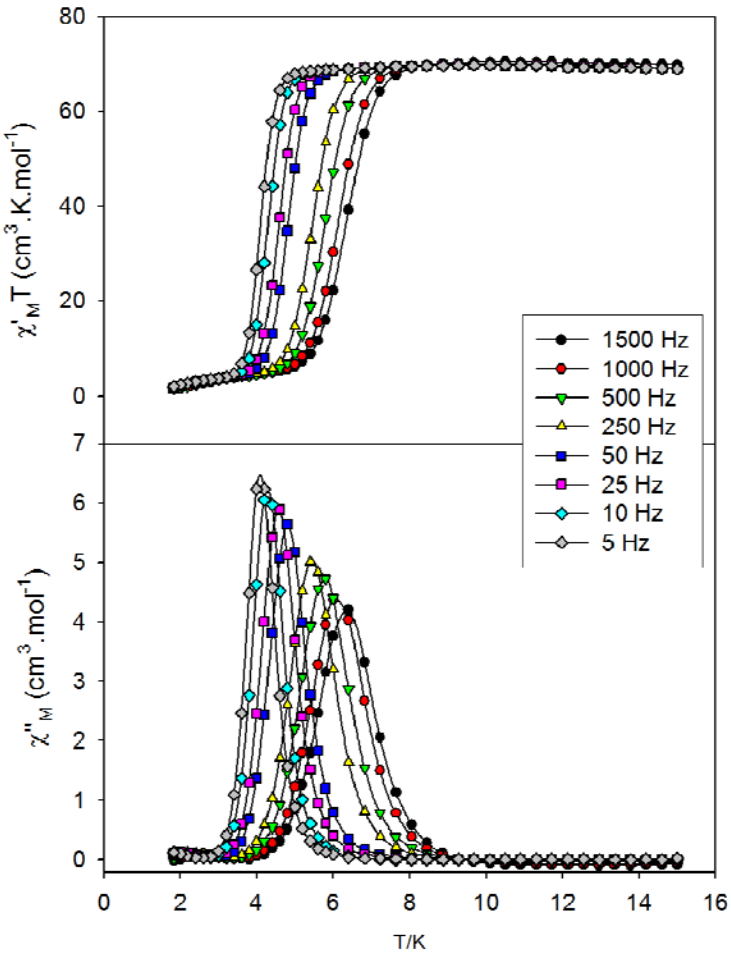

Figure S4. Plots of (top) in-phase $\chi'_M T$ vs T and (bottom) out-of-phase χ''_M vs T ac susceptibility data for **2**·8MeCN at the indicated ac oscillation frequencies.

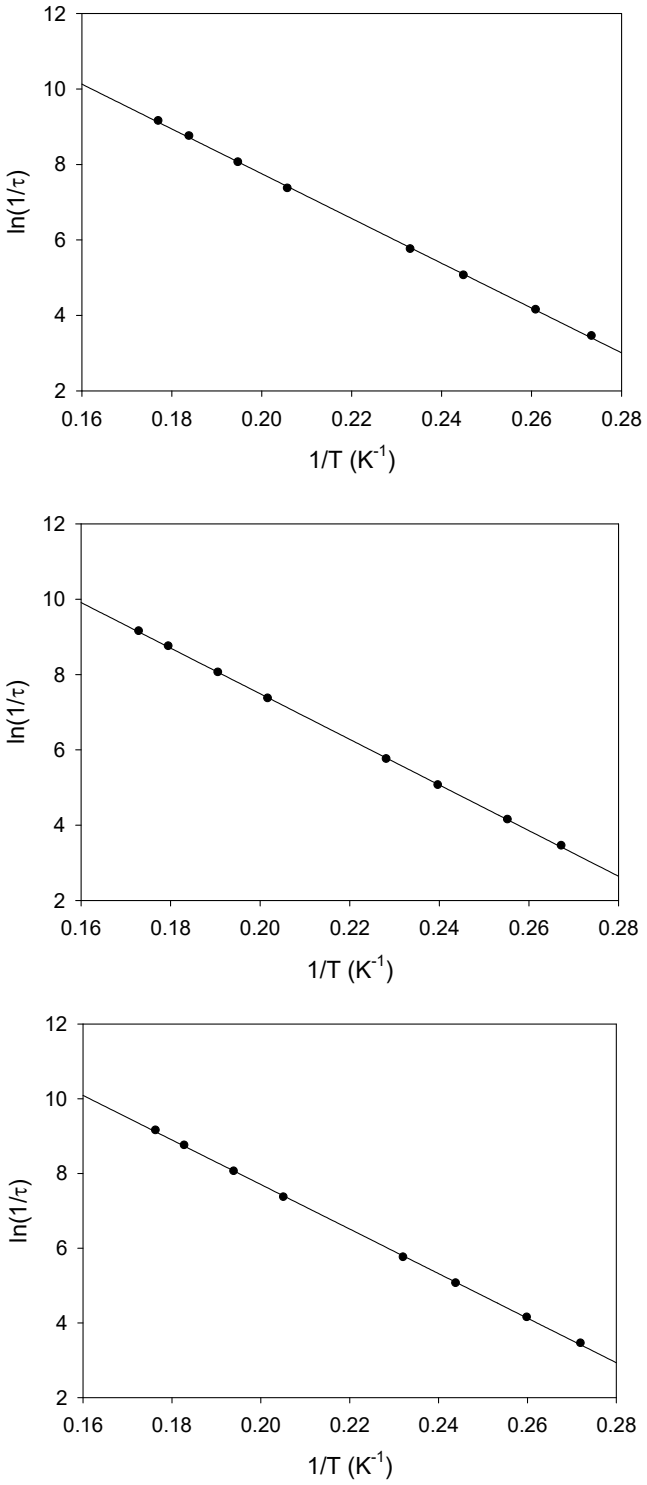

Figure S5. Arrhenius plots obtained using ac susceptibility data for (top) **2**·8MeCN (U_{eff} = 59.3 K, and pre-exponential $1/\tau_0 = 3.3\times10^8$ s^{-1}); (middle) vacuum-dried **2** (U_{eff} = 60.6 K and $1/\tau_0 = 3.3\times10^8$ s^{-1}); and (bottom) **2**·3H_2O after exposure of **2** to air for 32 h (U_{eff} = 59.6 K and $1/\tau_0 = 3.3\times10^8$ s^{-1}).

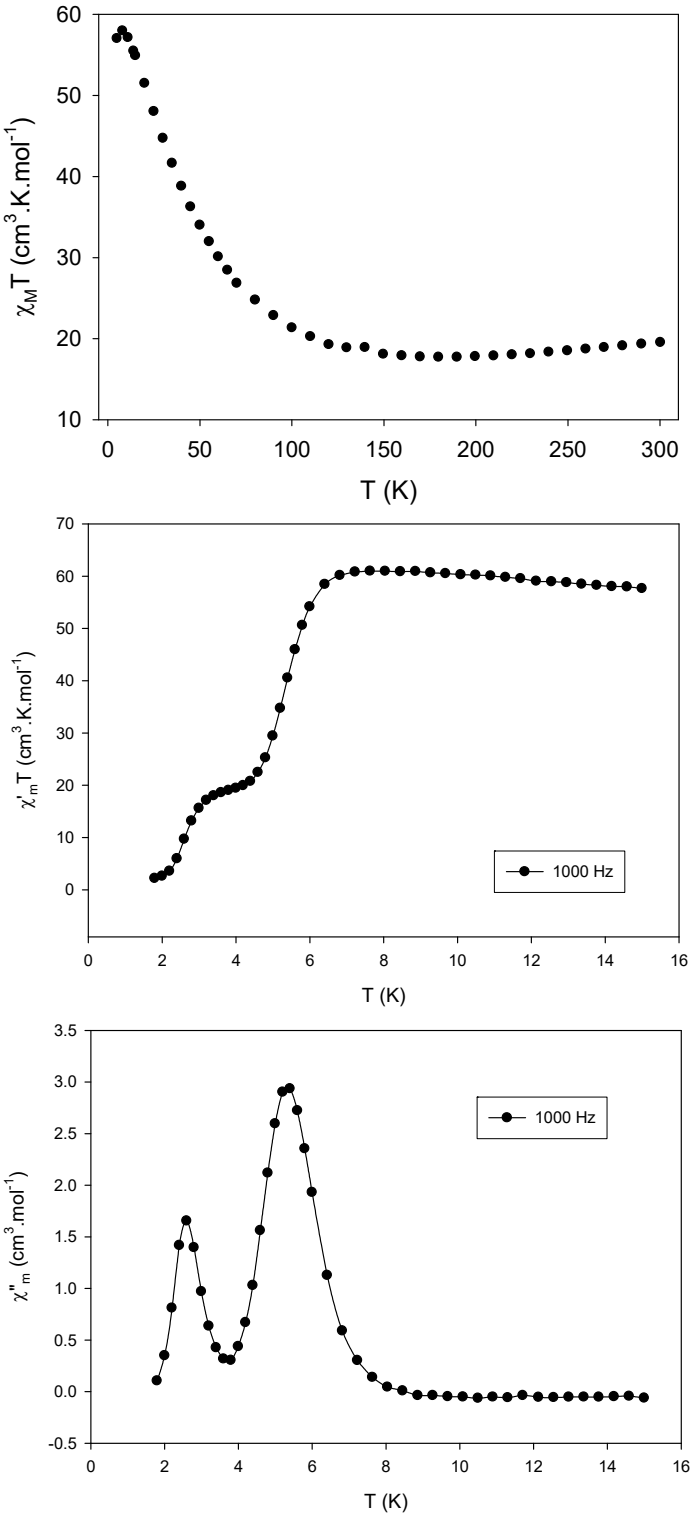

Figure S6. Dc and ac plots for **2**·3H_2O prepared by maintaining **2**·8MeCN exposed to air at ambient temperature and pressure for 10 days: (top) dc $\chi_M T$ vs T plot; (middle) ac in-phase $\chi'_M T$ vs T plot at 1000 Hz; and (bottom) ac out-of-phase χ''_M vs T plot at 1000 Hz.

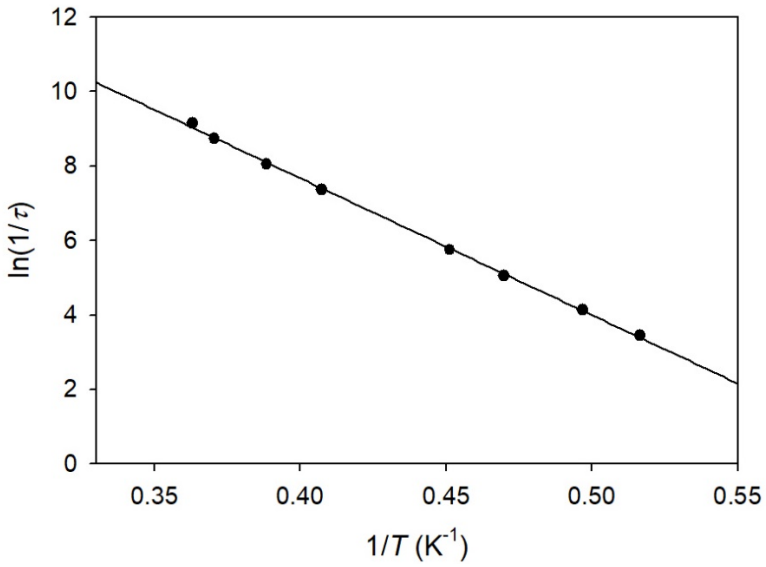

Figure S7. Arrhenius plot obtained using ac susceptibility data for the low-*T* **FR** JT isomer in **2**·3H$_2$O. The fit parameters were U_{eff} = 36.5 K, and pre-exponential $1/\tau_0 = 5.2\times10^9$ s^{-1})

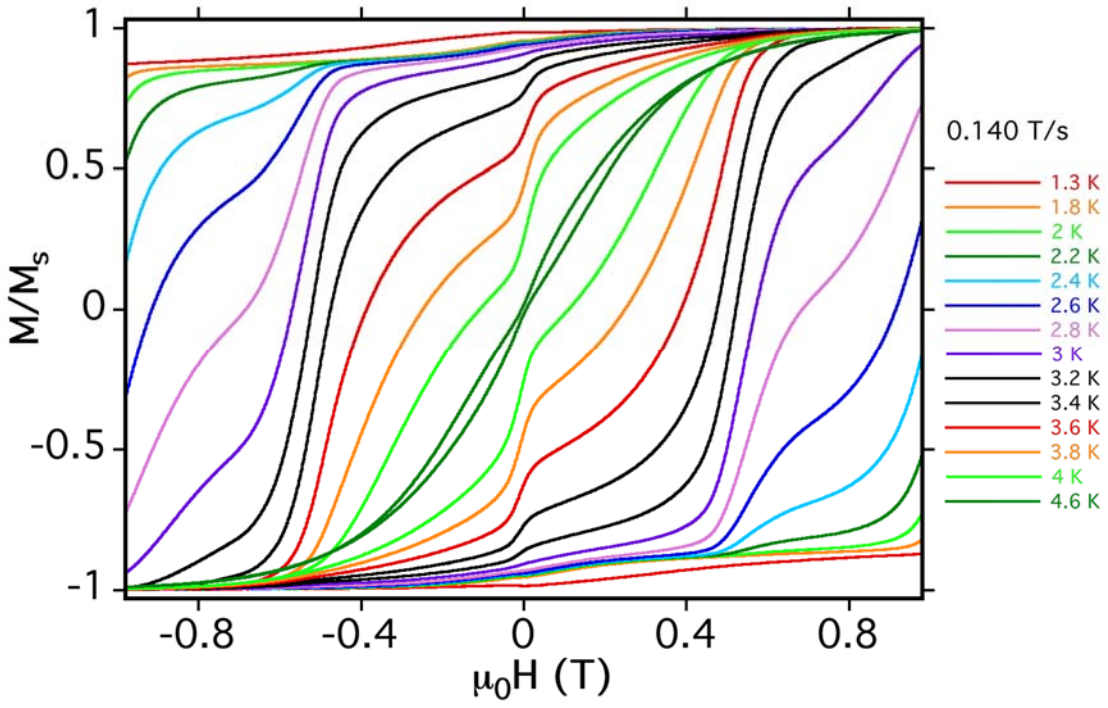

Figure S8. Magnetization (M) vs dc field hysteresis loops for a single crystal of **2**·8MeCN at the indicated field scan rate and temperatures. The magnetization was normalized to its saturation value, M_S.

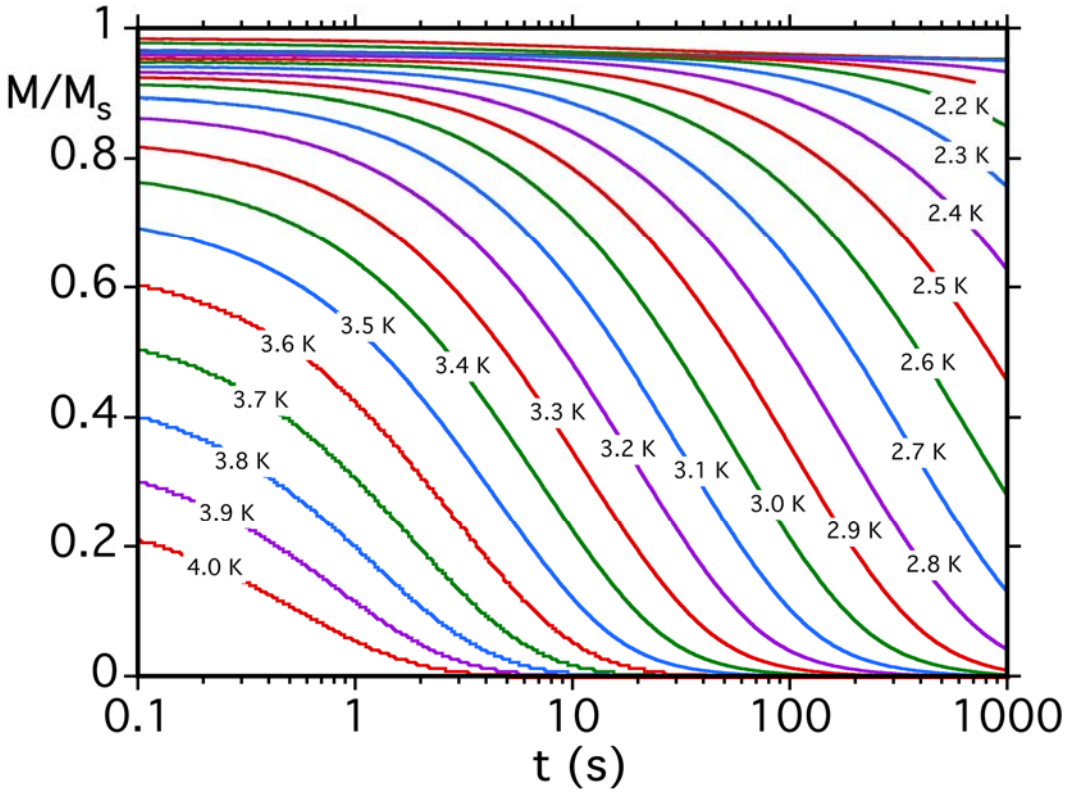

Figure S9. Magnetization (M) vs time (t) decay plots for a single crystal of **2**·8MeCN at the given temperatures. The magnetization was normalized to its saturation value, Ms.

Table S1. Root-mean-square deviations for overlaid cores of **1** and **2**.

	Atom Label	Deviation (Å)
1 vs **2** [a]	Mn1	0.050
	Mn2	0.278
	Mn3	0.112
	O1	0.044
	O2	0.063
	O3	0.078
2 vs **3** [b]	Mn1	0.025
	Mn2	0.045
	Mn3	0.098
	O1	0.020
	O2	0.091
	Mn1'	0.045
	Mn2'	0.177
	Mn3'	0.016
	O1'	0.025
	O2'	0.031
	Mn1"	0.029
	Mn2"	0.313
	Mn3"	0.094
	O1"	0.045
	O2"	0.022
	Mn1"'	0.050
	Mn2"'	0.211
	Mn3"'	0.046
	O1"'	0.024
	O2"'	0.097
	O3	0.066
	O3'	0.046
	O3"	0.062
	O3"'	0.112

[a] Weighted RMS Deviation = 0.132 Å
[b] Weighted RMS Deviation = 0.102 Å