

Supporting Information for

Discrete Polynuclear Manganese Nanorods: Syntheses, Crystal Structures and Magnetic Properties

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1. ^1H NMR spectra

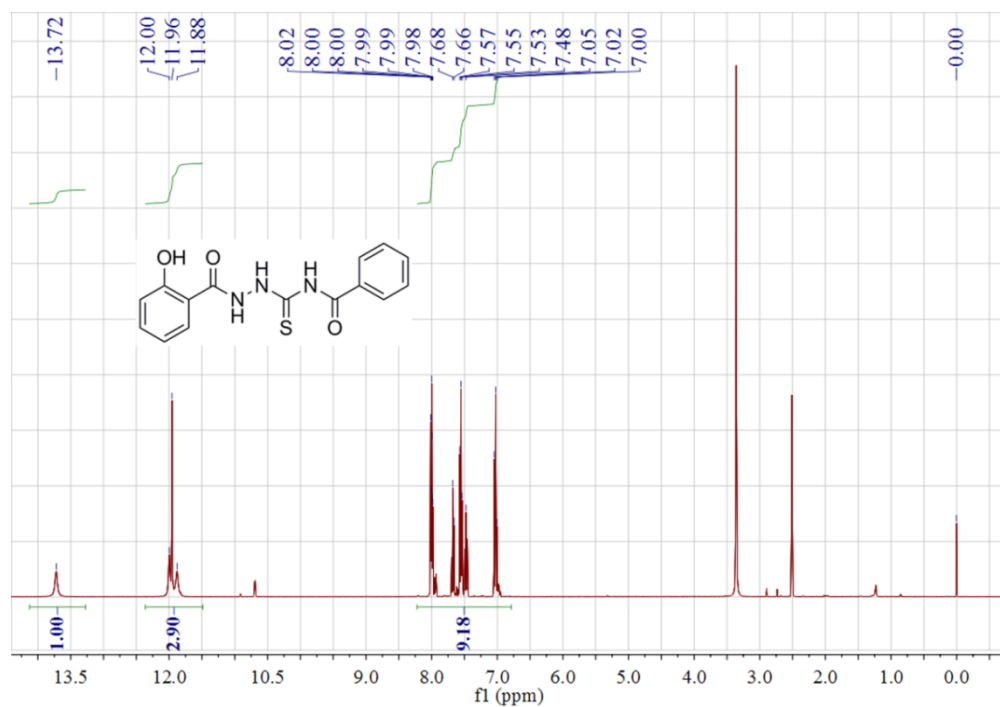


Figure S1. ^1H NMR spectrum of L1 in DMSO- d_6 (400 MHz, 293 K).

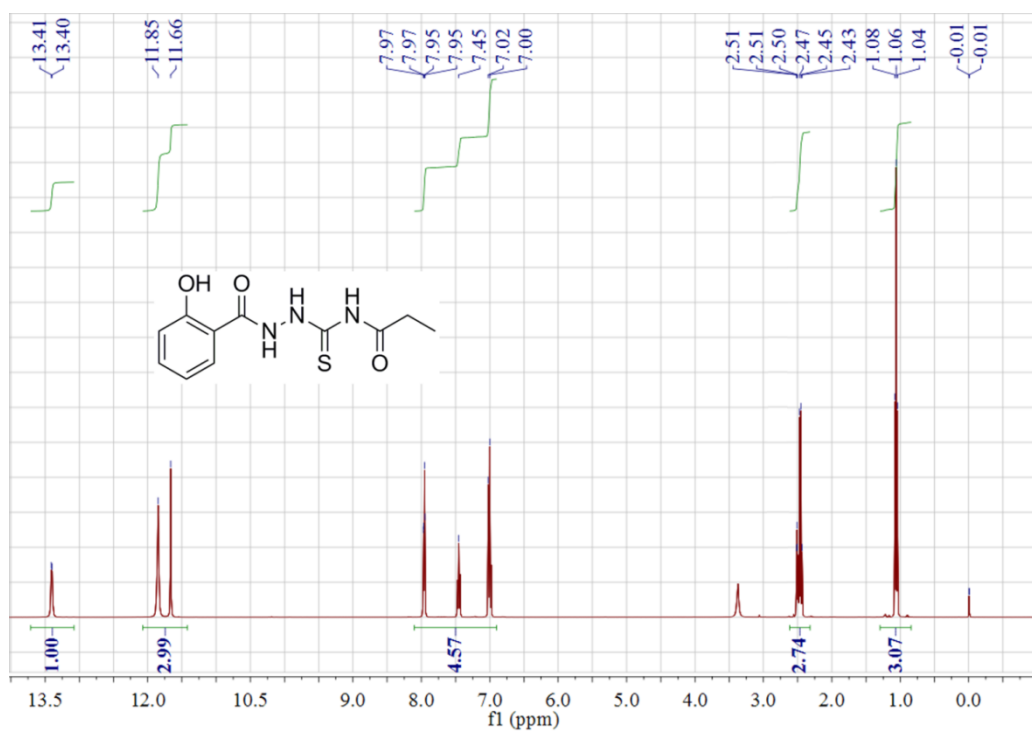


Figure S2. ^1H NMR spectrum of L2 in DMSO- d_6 (400 MHz, 293 K).

2. High-resolution mass spectra

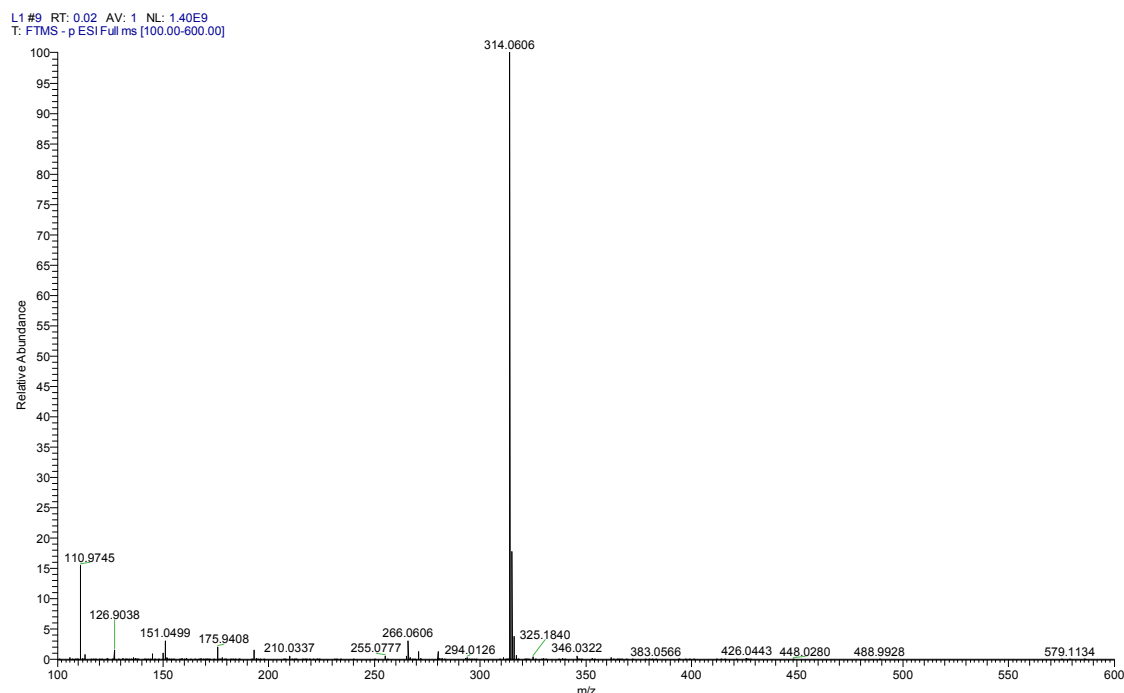


Figure S3. The High-resolution mass spectrum for L1

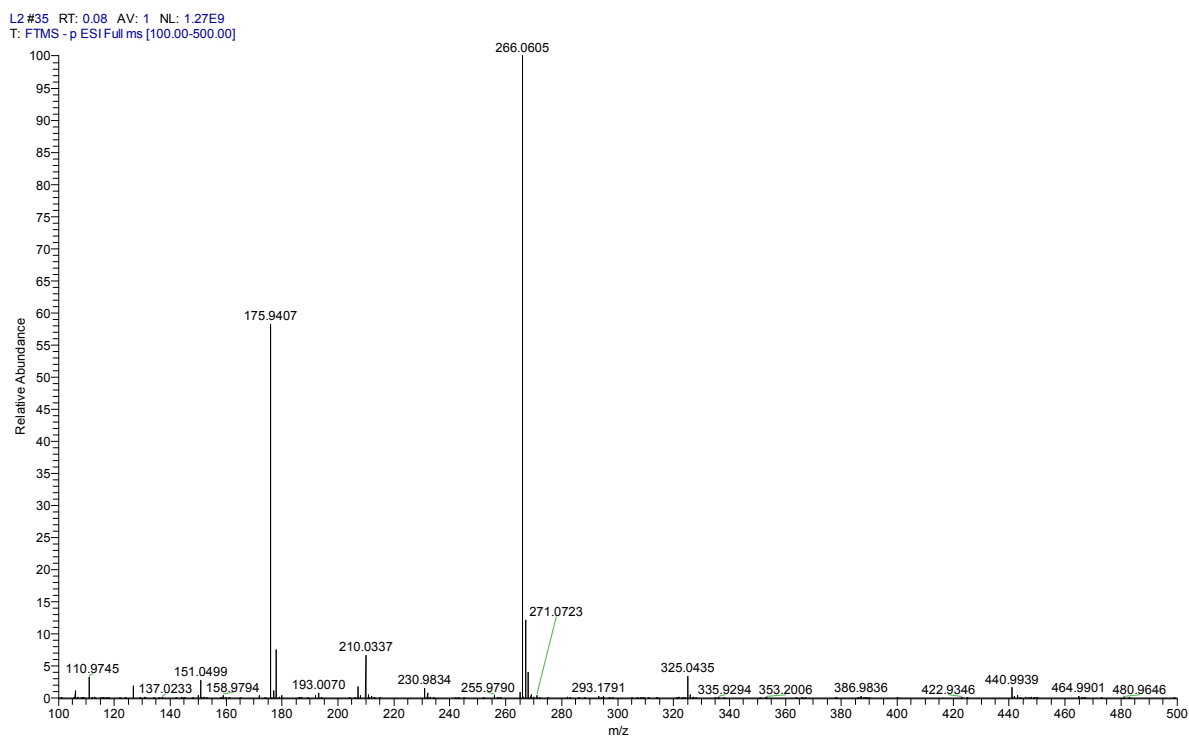
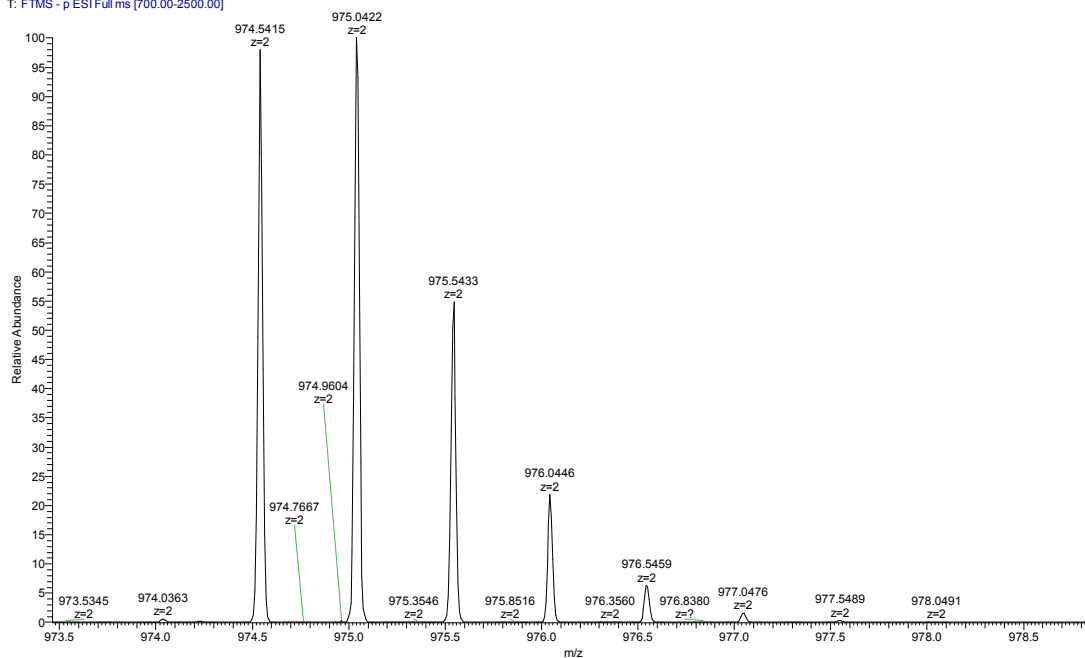


Figure S4. The High-resolution mass spectrum for L2

Mr=1947 140620113030 #8-24 RT: 0.04-0.11 AV: 17 NL: 2.99E8
T: FTMS - p ESI Full ms [700.00-2500.00]



Mr=1947 140620113030 #8-24 RT: 0.04-0.11 AV: 17 NL: 1.59E6
T: FTMS - p ESI Full ms [700.00-2500.00]

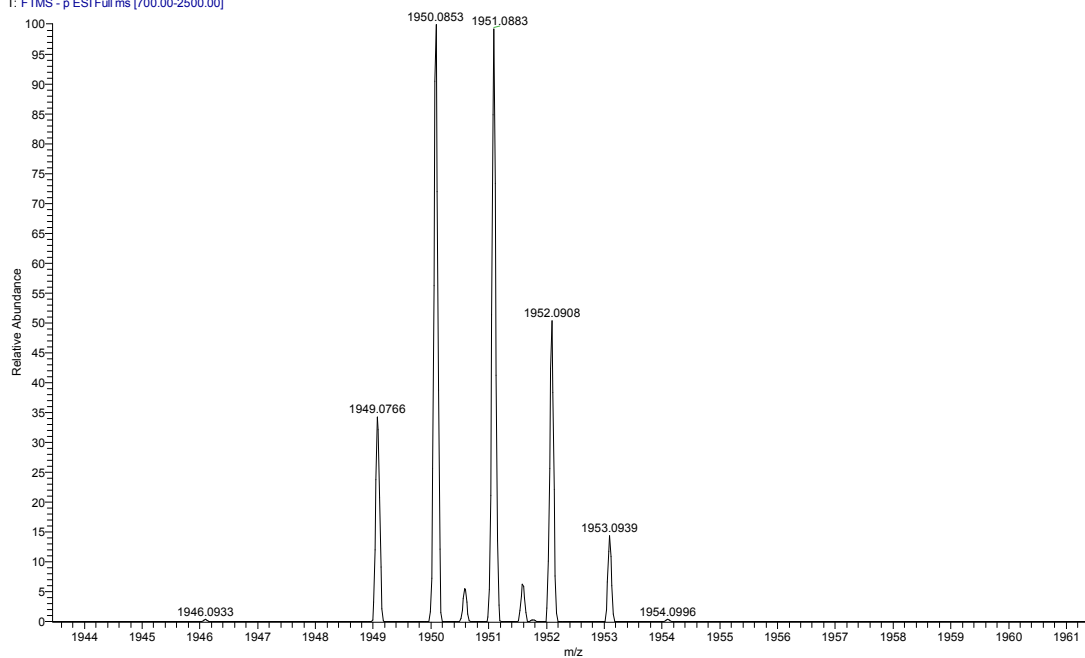


Figure S5. The High-resolution mass spectra for complex **1a** at 293 K.

3. Powder X-ray Diffraction Studies

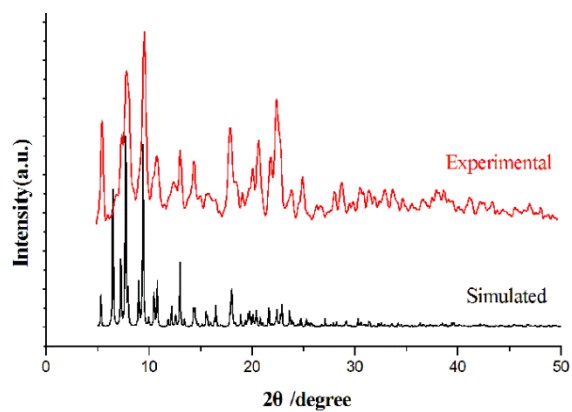


Figure S6. Comparison of the simulated and experimental PXRD for **1a**.

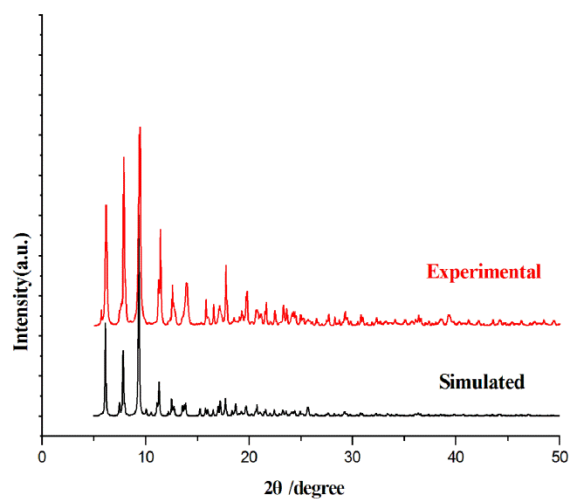


Figure S7. Comparison of the simulated and experimental PXRD for **1b**.

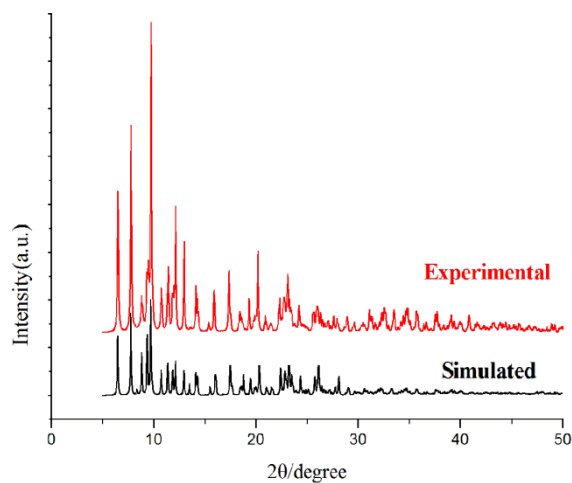


Figure S8. Comparison of the simulated and experimental PXRD for **2**.

4. Single Crystal Structures

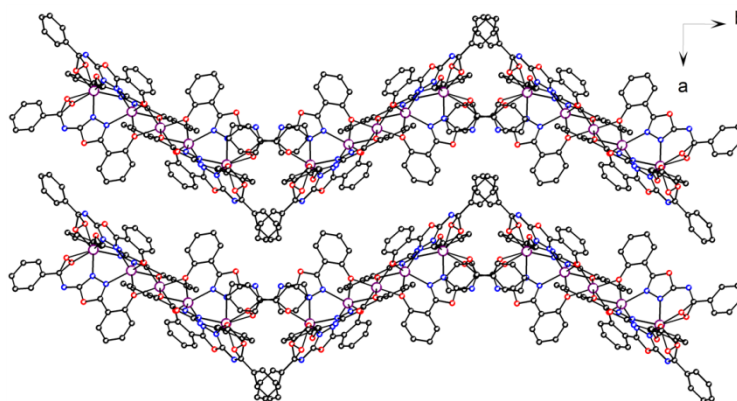


Figure S9. A packing diagram of complex **1a** along the *c* axis

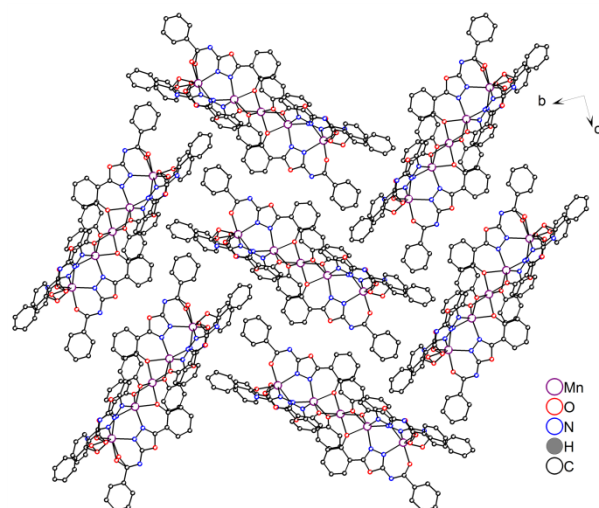


Figure S10. A packing diagram of complex **1a** along the *a* axis

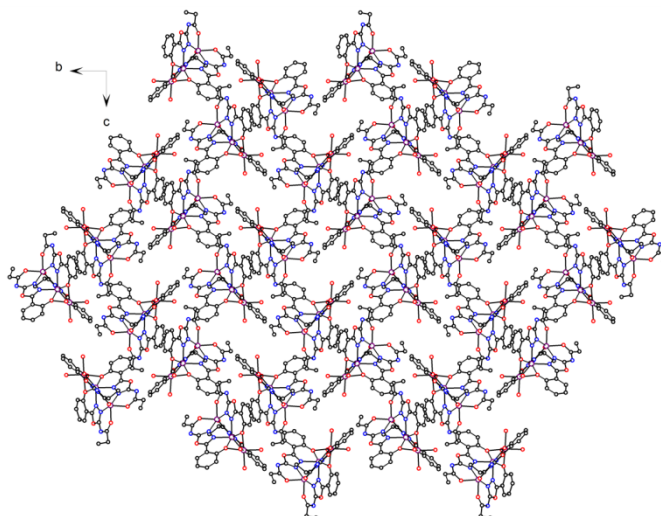


Figure S11. A packing diagram of complex **2** along the *a* axis

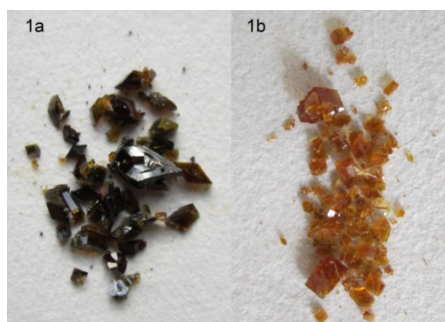


Figure S12. Photographic of the crystalline complex **1a** and **1b**

Table S1. Selected bond lengths (Å) for **1a**

Bonds	Dist. (Å)	Bonds	Dist. (Å)
Mn1—O7	2.180 (3)	Mn3—O3A	2.143 (6)
Mn1—O7 ⁱ	2.180 (3)	Mn3—O9A	2.143 (6)
Mn1—O4 ⁱ	2.195 (3)	Mn3—O9B	2.156 (12)
Mn1—O4	2.195 (3)	Mn3—N5	2.222 (4)
Mn1—O1	2.197 (3)	Mn3—N2	2.228 (4)
Mn1—O1 ⁱ	2.197 (3)	Mn3—N8	2.232 (4)
Mn2—O7	2.162 (3)	Mn4—O13	0.952 (9)
Mn2—O4	2.168 (3)	Mn4—O13 ⁱⁱ	0.952 (9)
Mn2—O1	2.180 (3)	Mn4—O10	2.125 (13)
Mn2—N1	2.215 (4)	Mn4—O10 ⁱⁱ	2.125 (13)
Mn2—N4	2.222 (4)	Mn4—O11	2.174 (12)
Mn2—N7	2.246 (4)	Mn4—O11 ⁱⁱ	2.174 (11)
Mn3—O6A	2.098 (6)	Mn4—O12 ⁱⁱ	2.250 (6)
Mn3—O3B	2.120 (12)	Mn4—O12	2.250 (6)
Mn3—O6B	2.130 (11)		

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+2, -y, -z+2$.

Table S2. Selected bond lengths (Å) for **1b**

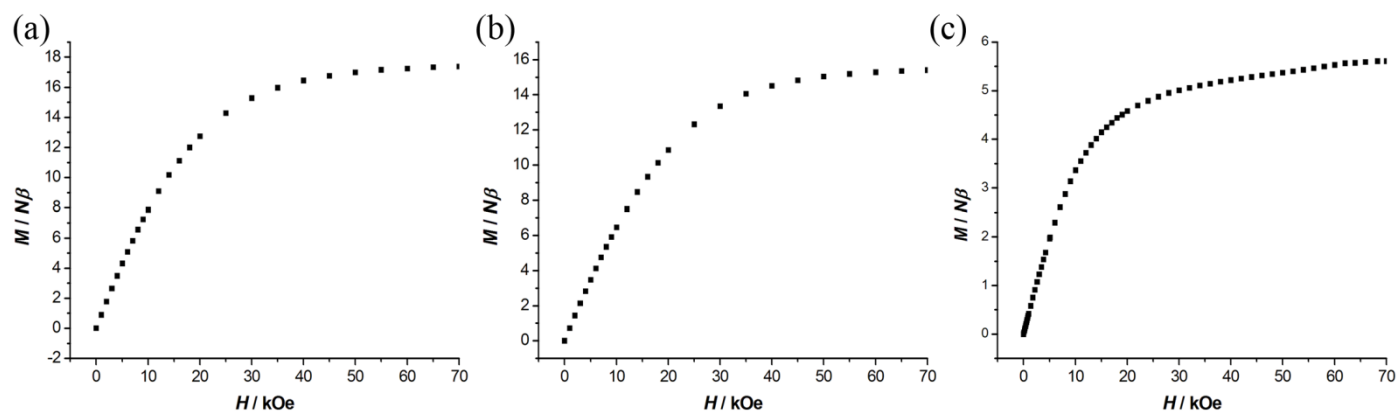
Bonds	Dist. (Å)	Bonds	Dist. (Å)
Mn1—O1 ⁱ	2.172 (3)	Mn2—N4	2.212 (4)
Mn1—O1	2.172 (3)	Mn2—N1	2.221 (4)
Mn1—O7 ⁱ	2.179 (3)	Mn2—N7	2.237 (3)
Mn1—O7	2.179 (3)	Mn3—O6	2.134 (3)
Mn1—O4 ⁱ	2.198 (3)	Mn3—O3	2.139 (3)
Mn1—O4	2.198 (3)	Mn3—O9	2.165 (3)
Mn1—Mn2	3.0033 (9)	Mn3—N8	2.238 (4)
Mn2—O4	2.160 (3)	Mn3—N5	2.246 (4)
Mn2—O7	2.175 (3)	Mn3—N2	2.252 (4)
Mn2—O1	2.176 (3)		

Symmetry code: (i) $-x+1, -y, -z+1$.

Table S3. Selected bond lengths (Å) for **2**

Bonds	Dist. (Å)	Bonds	Dist. (Å)
Mn1—O2	2.138 (7)	Mn2—N1	2.222 (8)
Mn1—O1	2.162 (8)	Mn2—N3	2.231 (9)
Mn1—O4	2.172 (7)	Mn2—N5	2.244 (8)
Mn1—O6	2.183 (7)	Mn3—O9	2.138 (8)
Mn1—O3	2.210 (8)	Mn3—O8	2.144 (8)
Mn1—O5	2.248 (7)	Mn3—O7	2.153 (9)
Mn1—Mn2	3.025 (2)	Mn3—N2	2.227 (9)
Mn2—O4	2.155 (7)	Mn3—N6	2.231 (9)
Mn2—O5	2.173 (7)	Mn3—N4	2.273 (9)
Mn2—O6	2.188 (7)		

5. Field-dependent magnetization

**Figure S13.** Field-dependent magnetizations of **1a** (a), **1b** (b) and **2** (c) at 2 K.