Electronic Supplementary Information

1D Chains from Mn₆ Single-Molecule Magnet Building Blocks

Leigh F. Jones,^a Allesandro Prescimone,^a Marco Evangelisti,^{*b} and Euan K. Brechin^{*a}

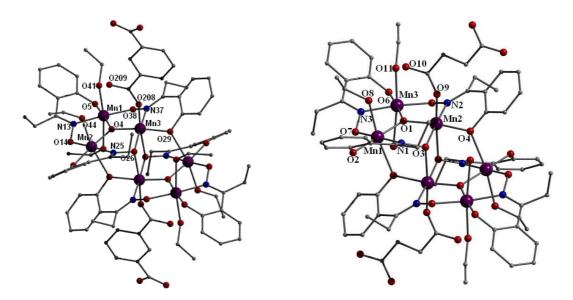


Figure SI1 Structures of the hexametallic building blocks in 1 (left) and 2 (right). H-atoms have been omitted for clarity.

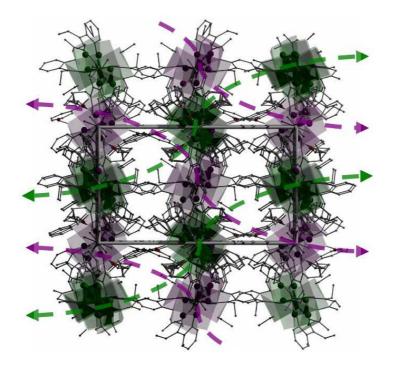


Figure SI2. Polyhedral representation of the packing of 1 in the crystal, viewed down the *ac* plane.

Supplementary Material (ESI) for Chemical Communications This journal is (c) The Royal Society of Chemistry 2009

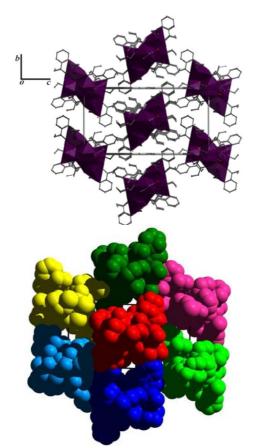
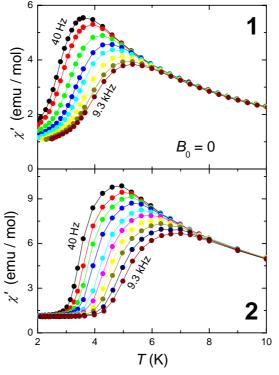


Figure SI3 (top) A Polyhedral representation of the packing observed in the crystal structure of **2** (H atoms have been omitted for clarity). The 1D chains comprising $[Mn_6]$ units propagate out of the page (along the *a* axis). (bottom) A space-fill representation also viewed along the *a* axis with each colour representing a different 1D chain.



SI4 Plots of temperature-dependencies of the in-phase χ' susceptibility for 1 (top) and 2 (bottom) for frequencies ranging from 40 to 9300 Hz.

Experimental Procedures

(1): $Mn(ClO_4)_2.6H_2O$ (0.25 g, 0.7 mmol), Et-saoH₂ (0.13 g, 0.7 mmol) and disodium isophthalate (0.15 g, 0.7 mmol) were dissolved in EtOH and added to this clear solution was 2 ml of a NEt₄(OH) solution (1 M in water) which resulted in the solution turning a dark red / black colour. The solution was stirred for 1 h and upon filtration and slow evaporation black crystals of **1** were obtained in 35 % yield after 4 days.

(2): $Mn(ClO_4)_2.6H_2O$ (0.7 mmol), Et-saoH₂ (0.7 mmol) and disodium succinate (0.7 mmol) were dissolved in EtOH and added to this clear solution was 2 ml of a NEt₄(OH) solution (1 M in water) which resulted in the solution turning a dark red / black colour. The solution was stirred for 1 h and upon filtration and slow evaporation black crystals of **1** were obtained in 30 % yield after 5 days.

Table SI1: Selected bond lengths (Å) and angles (°) for 1.

$\begin{array}{l} Mn (1) - 0 (4) \\ Mn (1) - 0 (5) \\ Mn (1) - N (13) \\ Mn (1) - 0 (38) \\ Mn (1) - 0 (41) \\ Mn (1) - 0 (47) \\ Mn (2) - 0 (29) \# 1 \\ Mn (2) - 0 (4) \\ Mn (2) - 0 (14) \\ Mn (2) - 0 (14) \\ Mn (2) - 0 (17) \\ Mn (2) - 0 (17) \\ Mn (2) - 0 (26) \\ Mn (3) - 0 (29) \\ Mn (3) - 0 (208) \\ \end{array}$	1.877(4) 1.855(4) 1.995(5) 1.922(4) 2.215(4) 2.336(5) 2.444(4) 1.893(4) 1.898(4) 1.854(4) 1.979(5) 2.241(4) 2.453(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 1.979(5) 2.241(4) 2.453(4) 1.994(4) 1.915(4) 2.025(5) 2.090(4)	$\begin{array}{l} Mn (101) - 0 (104) \\ Mn (101) - 0 (105) \\ Mn (101) - N (113) \\ Mn (101) - 0 (138) \\ Mn (101) - 0 (141) \\ Mn (101) - 0 (147) \\ Mn (102) - 0 (129) \#2 \\ Mn (102) - 0 (129) \#2 \\ Mn (102) - 0 (104) \\ Mn (102) - 0 (104) \\ Mn (102) - 0 (114) \\ Mn (102) - 0 (117) \\ Mn (102) - 0 (117) \\ Mn (102) - 0 (125) \\ Mn (102) - 0 (124) \\ Mn (103) - 0 (126) \#2 \\ Mn (103) - 0 (126) \\ Mn (103) - 0 (129) \\ Mn (103) - 0 (211) \\ \end{array}$	$\begin{array}{c} 1.886(4)\\ 1.890(4)\\ 2.002(6)\\ 1.925(4)\\ 2.240(5)\\ 2.258(5)\\ 2.412(4)\\ 3.2545(1)\\ 1.890(4)\\ 1.901(4)\\ 1.901(4)\\ 1.989(5)\\ 2.242(6)\\ 2.459(4)\\ 1.966(4)\\ 1.966(4)\\ 1.986(5)\\ 2.109(4)\\ \end{array}$	O(4) - Mn(1) - O(5) O(4) - Mn(1) - O(38) O(5) - Mn(1) - O(38) N(13) - Mn(1) - O(38) O(4) - Mn(1) - O(41) O(5) - Mn(1) - O(41) O(5) - Mn(1) - O(41) O(38) - Mn(1) - O(41) O(4) - Mn(1) - O(47) O(5) - Mn(1) - O(47) O(5) - Mn(1) - O(47) O(38) - Mn(1) - O(47) O(38) - Mn(1) - O(47) O(38) - Mn(1) - O(47) O(29) #1 - Mn(2) - O(14) O(29) #1 - Mn(2) - O(14) O(29) #1 - Mn(2) - O(17) O(14) - Mn(2) - O(17) O(14) - Mn(2) - N(25) O(4) - Mn(2) - N(25)	$\begin{array}{c} 176.60(18)\\ 91.48(17)\\ 90.09(18)\\ 176.23(19)\\ 89.63(16)\\ 93.29(18)\\ 90.19(19)\\ 93.50(17)\\ 89.09(17)\\ 89.09(17)\\ 87.75(18)\\ 80.87(19)\\ 95.45(17)\\ 170.99(18)\\ 86.75(14)\\ 98.54(16)\\ 92.63(17)\\ 89.40(16)\\ 175.38(17)\\ 90.45(18)\\ 79.78(16)\\ 88.33(18)\\ \end{array}$	O(29) #1-Mn(2) - O(44) O(4) -Mn(2) - O(44) O(14) -Mn(2) - O(44) O(17) -Mn(2) - O(44) O(25) -Mn(2) - O(44) O(26) #1-Mn(3) - O(26) O(26) #1-Mn(3) - O(26) O(26) #1-Mn(3) - O(29) O(26) #1-Mn(3) - O(29) O(26) -Mn(3) - O(29) O(26) -Mn(3) - O(29) O(26) #1-Mn(3) - N(37) O(26) -Mn(3) - N(37) O(26) -Mn(3) - N(37) O(26) -Mn(3) - O(208) O(26) -Mn(3) - O(208) O(29) -Mn(3) - O(208) O(29) -Mn(3) - O(208) N(37) -Mn(3) - O(208) Mn(2) - O(4) -Mn(1)	$166.99(16) \\88.70(17) \\93.83(19 \\94.52(18) \\87.91(18) \\87.91(18) \\84.86(15) \\85.61(15) \\89.84(17) \\84.81(14) \\169.60(16) \\90.56(16) \\84.89(16) \\84.89(16) \\84.87(18) \\170.49(17) \\174.92(16) \\100.10(17) \\95.43(17) \\89.03(18) \\90.20(17) \\94.07(18) \\118.49(19) \\$
				O(14) - Mn(2) - N(25)	178.03(19)	Mn(2) = O(4) = Mn(3)	120.9(2)
				O(17) - Mn(2) - N(25)	88.49(19)	Mn(1) = O(4) = Mn(3)	120.0(2)

Table SI2: Selected bond lengths (Å) and angles (°) for 2.

Mn(1)-0(28)#1	2.4067(18)	O(28)#1-Mn(1)-O(29)#1	83.46(7)	N(27) - Mn(2) - O(29)	80.83(7)
Mn(1)-0(29)#1	1.9090(17)	O(28)#1-Mn(1)-O(4)	84.68(7)	0(4)-Mn(2)-0(45)	87.98(7)
Mn(1) = O(4)	1.8676(17)	O(29)#1-Mn(1)-O(4)	167.75(8)	0(16)-Mn(2)-0(45)	93.36(8)
Mn(1) = O(28)	1.9534(17)	O(28)#1-Mn(1)-O(28)	85.20(7)	O(17) - Mn(2) - O(45)	90.99(8)
Mn(1) - N(39)	2.009(2)	O(29)#1-Mn(1)-O(28)	91.78(7)	N(27)-Mn(2)-0(45)	88.99(8)
Mn(1) = O(41)	2.0877(19)	O(4) - Mn(1) - O(28)	90.24(7)	0(29)-Mn(2)-0(45)	169.44(7)
Mn(2) = O(4)	1.8956(17)	0(28)#1-Mn(1)-N(39)	88.07(8)	O(4) - Mn(3) - O(5)	174.91(9)
Mn(2)-0(16)	1.9129(18)	0(29)#1-Mn(1)-N(39)	88.07(8)	O(4) - Mn(3) - N(15)	88.44(8)
Mn(2)-0(17)	1.8728(17)	O(4) - Mn(1) - N(39)	88.52(8)	O(5) - Mn(3) - N(15)	88.38(8)
Mn(2) - N(27)	1.986(2)	0(28)-Mn(1)-N(39)	173.25(9)	O(4) - Mn(3) - O(40)	91.59(7)
Mn(2)-0(29)	2.3483(17)	O(28)#1-Mn(1)-O(41)	174.80(7)	0(5)-Mn(3)-0(40)	91.11(7)
Mn(2)-0(45)	2.218(2)	O(29)#1-Mn(1)-O(41)	91.89(7)	N(15)-Mn(3)-O(40)	173.29(9)
Mn(3)-0(4)	1.8688(17)	O(4) - Mn(1) - O(41)	100.08(7)	O(4) - Mn(3) - O(51)	85.44(8)
Mn (3) -0(5)	1.8770(18)	O(28)-Mn(1)-O(41)	92.64(7)	0(5)-Mn(3)-0(51)	90.08(10)
Mn(3) - N(15)	2.004(2)	N(39) - Mn(1) - O(41)	94.12(8)	N(15)-Mn(3)-O(51)	79.72(9)
Mn(3)-0(40)	1.9222(19)	O(4) - Mn(2) - O(16)	91.06(7)	O(4) - Mn(3) - O(48)	93.29(8)
Mn(3)-0(51)	2.382(3)	O(4) - Mn(2) - O(17)	176.14(8)	0(5)-Mn(3)-0(48)	90.86(9)
Mn(3)-0(48)	2.204(2)	O(16)-Mn(2)-O(17)	92.72(8)	N(15)-Mn(3)-O(48)	93.36(8)
		O(4) - Mn(2) - N(27)	88.28(8)	0(40)-Mn(3)-0(51)	93.59(9)
		O(16) - Mn(2) - N(27)	177.54(9)	0(40)-Mn(3)-0(48)	93.34(8)
		O(17) - Mn(2) - N(27)	87.98(8)	0(51)-Mn(3)-0(48)	172.99(9)
		O(4) - Mn(2) - O(29)	88.91(7)	Mn(2) = O(4) = Mn(3)	119.67(9)
		O(16) -Mn(2) -O(29)	96.79(7)	Mn(2) = O(4) = Mn(1)	119.77(8)
		0(17)-Mn(2)-0(29)	91.43(7)	Mn(3) = O(4) = Mn(1)	120.29(9)