

Electronic Supplementary Information

Homo- and Heterometallic Planes, Chains and Cubanes

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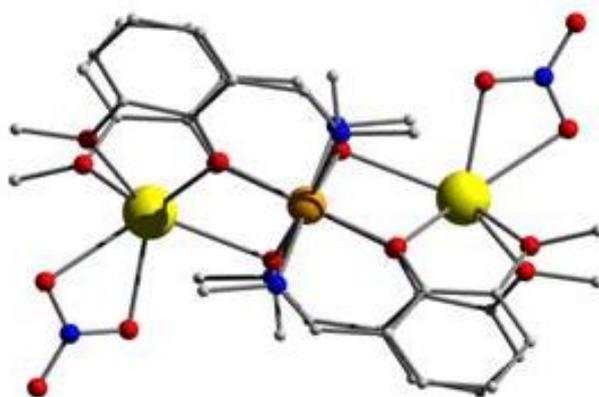


Figure S1 Side views along the plane of the $[\text{Na}_2\text{M}_2]$ butterfly cores in **1**. Colour codes: Brown (Fe), Yellow (Na), Red (O), Blue (N), Grey (C). Hydrogen atoms have been omitted for clarity.

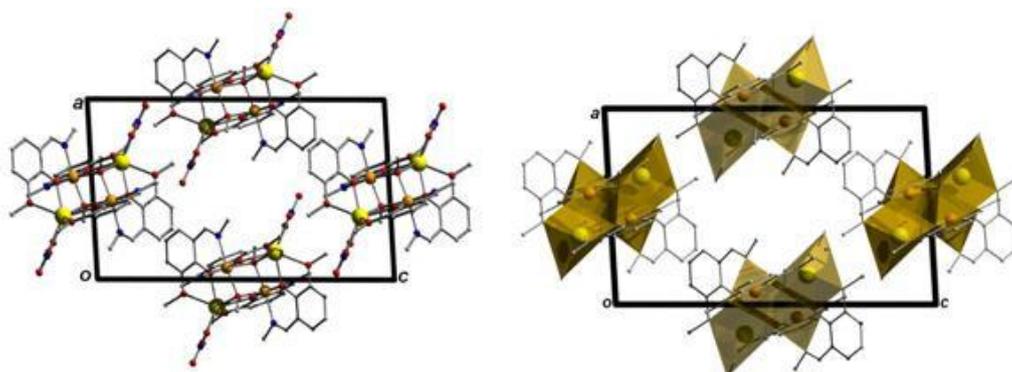


Fig. S2 Ball and stick (left) and polyhedral (right) crystal packing schematics of **1** as viewed along the $[0\ 1\ 0]$ face of the cell. Hydrogen atoms have been omitted for clarity. Complex **2** packs in the same way.

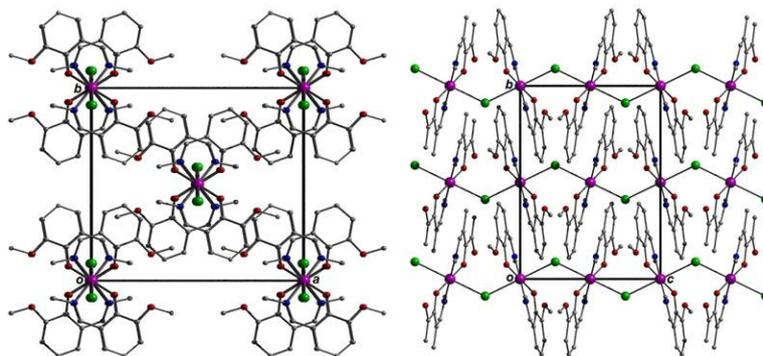


Figure S3: Crystal packing in **4** as observed down the *c* (left) *a* axis (right) respectively. Colour codes: Pink (Mn), Green (Cl), Red (O), Blue (N), Grey (C). Hydrogen atoms have been omitted for clarity.

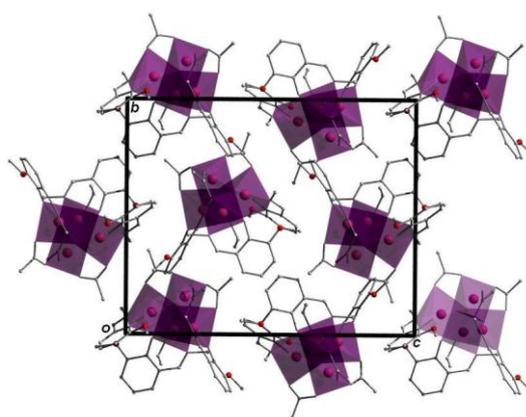


Figure S4: Polyhedral representation of the crystal packing in **5** observed down the *a* axis. Hydrogen atoms have been omitted for clarity.

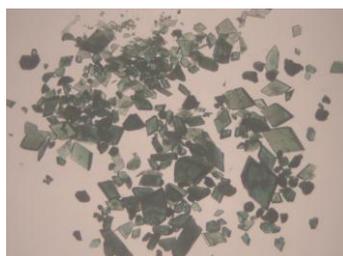


Fig. S5 Microscope image of crystalline sample of $[\text{Ni}_4(\mu_3\text{-OMe})_4(\text{L}_2)_4(\text{MeOH})_4]$ (**6**).

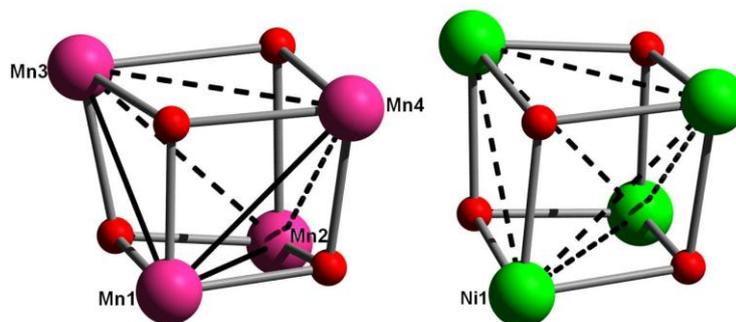


Fig. S6 (left) Schematic representing the 2-J model employed to fit the magnetic data in **5** (solid lines = J_1 , dashed lines = J_2). (right) 1-J model utilised in fitting magnetic data from complex **6** (dashed line = J_1). For specific spin Hamiltonian parameters see main text.

Table S1: Selected bond length (Å) and angles (°) obtained from complexes **1-3**

Bond lengths (Å) / angles (°)	1	Bond lengths (Å) / angles (°)	2	Bond lengths (Å) / angles (°)	3
Fe1-O2	1.944(6)	Ni1-O2	2.0056(13)	Ni1-O1	2.058(7)
Fe1-O4	1.956(6)	Ni1-O4	2.0038(12)	Ni1-N1	2.106(10)
Fe1-O5	2.015(6)	Ni1-N1	2.2084(15)	Ni2-O4	2.043(7)
Fe1-O5'	2.032(6)	Ni1'-N1	2.1758(15)	Ni2-N2	2.104(9)
Fe1-N1	2.152(7)	Ni1 N4	2.0771(15)		
Fe1-N2	2.152(7)	Ni1 N5	2.0609(15)	Na1-O1	2.686(9)
				Na1-O1'	2.265(8)
Na1-O1	2.427(7)	Na1-O1	2.4470(15)	Na1-O2	2.329(9)
Na1-O2	2.350(7)	Na1-O2	2.2501(14)	Na1-O3	2.343(9)
Na1-O3	2.398(7)	Na1-O3	2.4611(15)	Na1-O4	2.262(8)
Na1-O4	2.371(7)	Na1-O4	2.2640(14)	Na1-O4'	2.618(8)
Na1-O5	2.604(7)	Na1-N1	2.5790(17)		
Na1-O6	2.545(9)	Na1-N6	2.4558(19)	Ni1-O1-Na1	109.6(3)
Na1-O8	2.374(10)			Ni2-O4-Na1	108.9(3)
		Ni1-N1-Na1	91.95(6)	Na1-O1-Na1'	81.8(3)
Fe1-O5-Fe1'	101.4(3)	Ni1'-N1-Na1	93.14(6)	Na1-O4-Na1'	83.4(3)
Fe1-O2-Na1	108.1(3)	Ni1-O2-Na1	108.28(6)		
Fe1-O5-Na1	97.1(2)	Ni1'-O4-Na1	108.37(6)		
Fe1-O4-Na1	105.4(3)	Ni1-N1-Ni1'	99.75(6)		

Table S2: Selected bond length (Å) obtained from complex **4**

Bond lengths (Å)	4
Mn1-O1	1.854(2)
Mn1-N1	2.030(3)
Mn1-Cl1	2.676(7)
Mn...Mn	4.845

Table S3: Selected bond length (Å) and angles (°) obtained from complexes **5** and **6**.

Bond lengths (Å) / angles (°)		Bond lengths (Å) / angles (°)	
Mn1-O8	1.975(3)	Mn1-O16-Mn3	94.78(13)
Mn1-O10	1.949(3)	Mn1-O16-Mn2	94.29(13)
Mn1-O11	1.954(3)	Mn1-O14-Mn2	95.79(14)
Mn1-O14	1.854(3)	Mn1-O14-Mn4	95.55(13)
Mn1-O15	1.868(3)	Mn1-O15-Mn3	96.18(13)
Mn1-O16	1.885(3)	Mn1-O15-Mn4	93.56(13)
		Mn2-O16-Mn3	109.87(14)
Mn2-O1	1.880(3)	Mn2-O13-Mn3	90.56(12)
Mn2-O9	2.231(3)	Mn2-O13-Mn4	88.78(11)
Mn2-O13	2.241(3)	Mn2-O14-Mn4	108.14(14)
Mn2-O14	1.936(3)	Mn3-O13-Mn4	91.53(12)
Mn2-O16	1.950(3)	Mn3-O15-Mn4	110.86(15)
Mn2-N1	1.996(4)		
		(6)	
Mn3-O5	1.872(3)	Ni1-O1	2.090(4)
Mn3-O12	2.236(3)	Ni1-O2	2.034(3)
Mn3-O13	2.250(4)	Ni1-O2'	2.066(4)
Mn3-O15	1.925(3)	Ni1-O2''	2.022(4)
Mn3-O16	1.949(3)	Ni1-O3	1.991(3)
Mn3-N3	2.024(4)	Ni1-N1	2.004(3)
Mn4-O3	1.856(3)	Ni1-O2-Ni1'	97.93(14)
Mn4-O7	2.182(3)	Ni1-O2-Ni1''	96.51(14)
Mn4-O13	2.223(3)	Ni1-O2-Ni1'''	98.36(16)

Mn4-O14	1.921(3)		
Mn4-O15	1.967(3)		
Mn4-N2	2.018(4)		

Table SI4: BVS Calculations for the Manganese centres in **5** (figures to 2 d.p)

Calculated as:	Mn1	Mn2	Mn3	Mn4
Mn ^{III}	3.99	3.01	2.99	3.09
Mn ^{IV}	3.91	2.96	2.94	3.03

X-ray diffraction details on the collection of 1-6

All hydrogen atoms in all complexes were placed in calculated positions. All non-hydrogen atoms were refined anisotropically. In complex **1** the MeOH solvent molecules were modelled to be disordered over two sites at 50:50 occupancy. DFIX restraints were also put in place between the C and O atoms in both disordered MeOH solvent molecules.