Electronic Supplementary Information

Structural Influences on the Exchange Coupling and Zero-Field Splitting in the Single-Molecule Magnet $[Mn^{III}_6Mn^{III}]^{3+}$

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Fig. S1. Thermal ellipsoid plots of the two independent fragments ((a) and (b)) of $[Mn^{III}_{6}Mn^{III}]^{3+}$ molecules in the asymmetric unit in crystals of **1** with the numbering scheme used. Thermal ellipsoids are drawn at the 50 % probability level; hydrogen atoms are omitted for clarity.

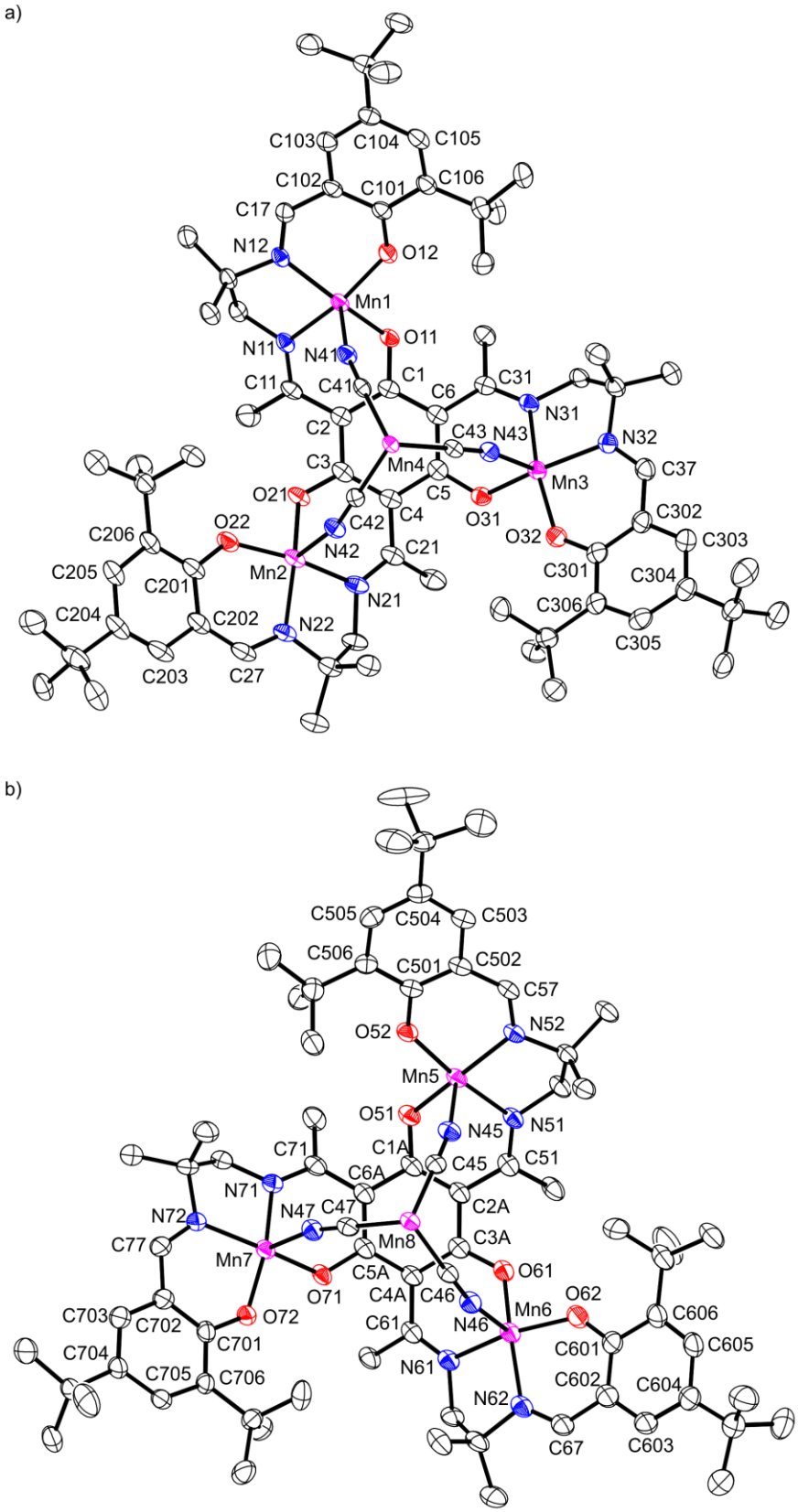

Fig. S2. Thermal ellipsoid plots of the two independent fragments ((a) and (b)) of $[Mn^{III}_6Mn^{III}]^{3+}$ molecules in the asymmetric unit in crystals of **2** with the numbering scheme used. Thermal ellipsoids are drawn at the 50 % probability level; hydrogen atoms are omitted for clarity.

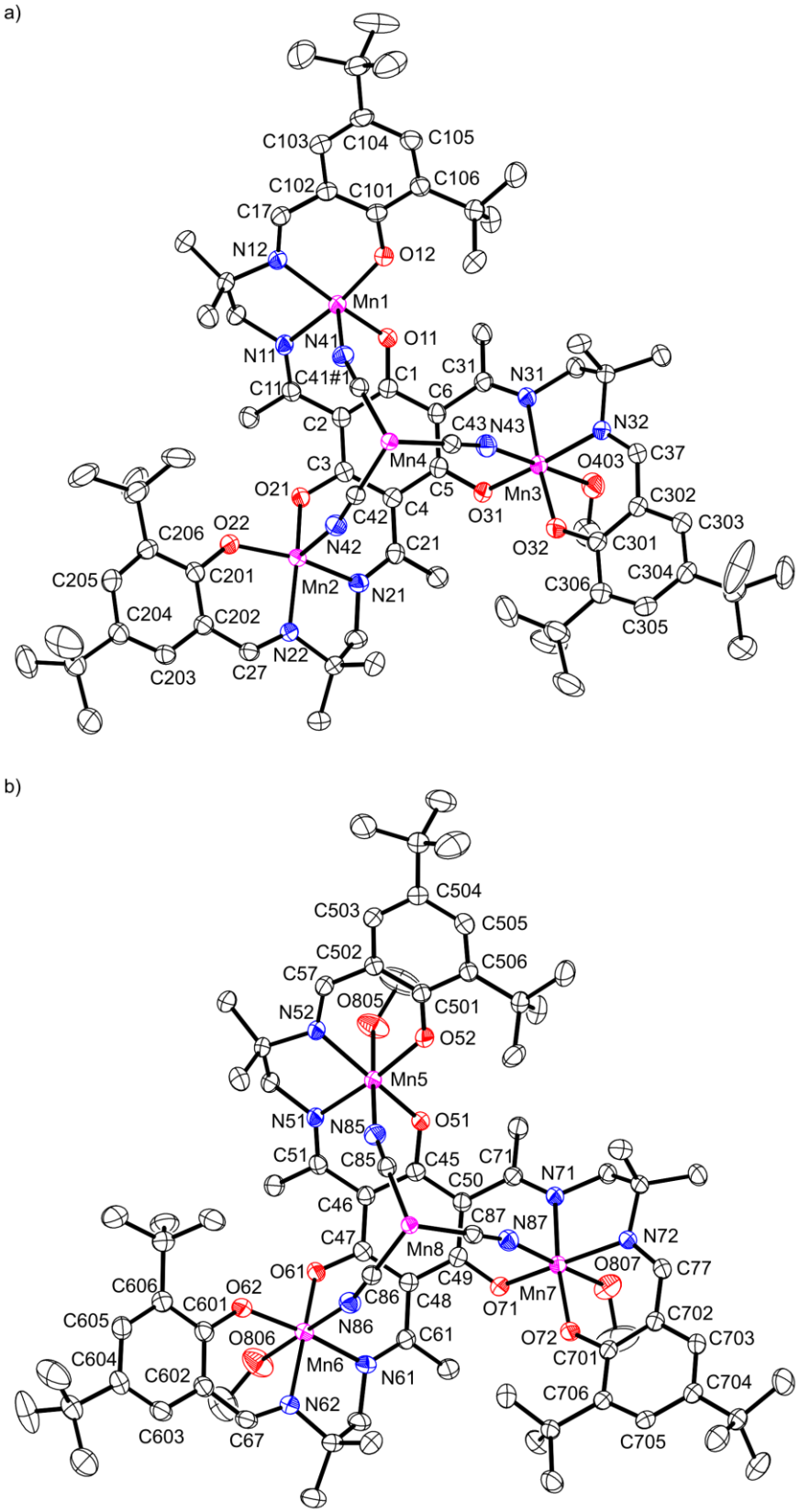

Fig. S3. Thermal ellipsoid plot of the fragment of the **$[Mn^{III}_6Mn^{III}]^{3+}$** molecule in the asymmetric unit in crystals of **3** with the numbering scheme used. Thermal ellipsoids are drawn at the 50 % probability level; hydrogen atoms are omitted for clarity.

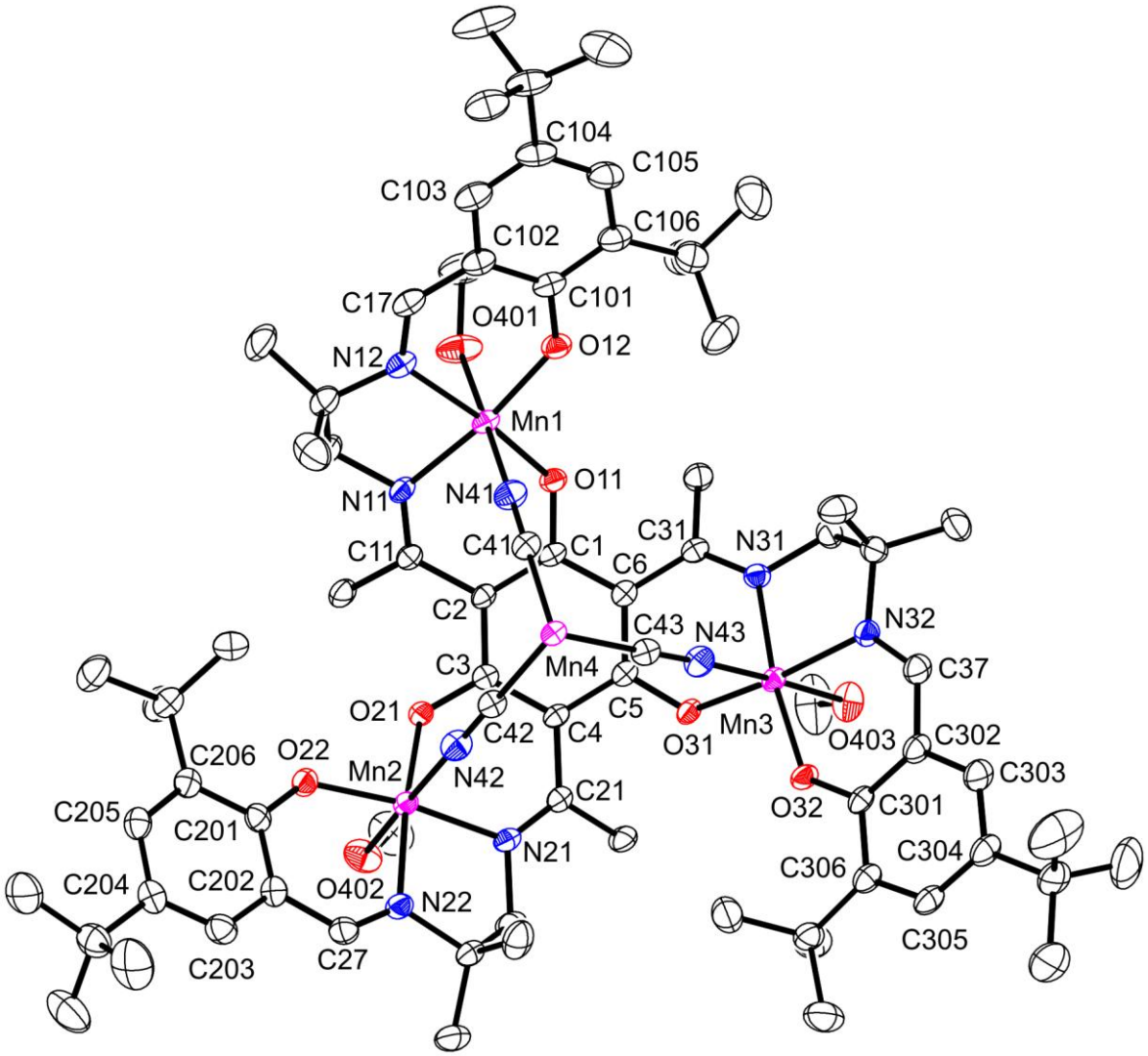

Fig. S4. Thermal ellipsoid plot of the fragment of the $[Mn^{III}_6Mn^{III}]^{3+}$ molecule in the asymmetric unit in crystals of **4** with the numbering scheme used. Thermal ellipsoids are drawn at the 50 % probability level; hydrogen atoms are omitted for clarity.

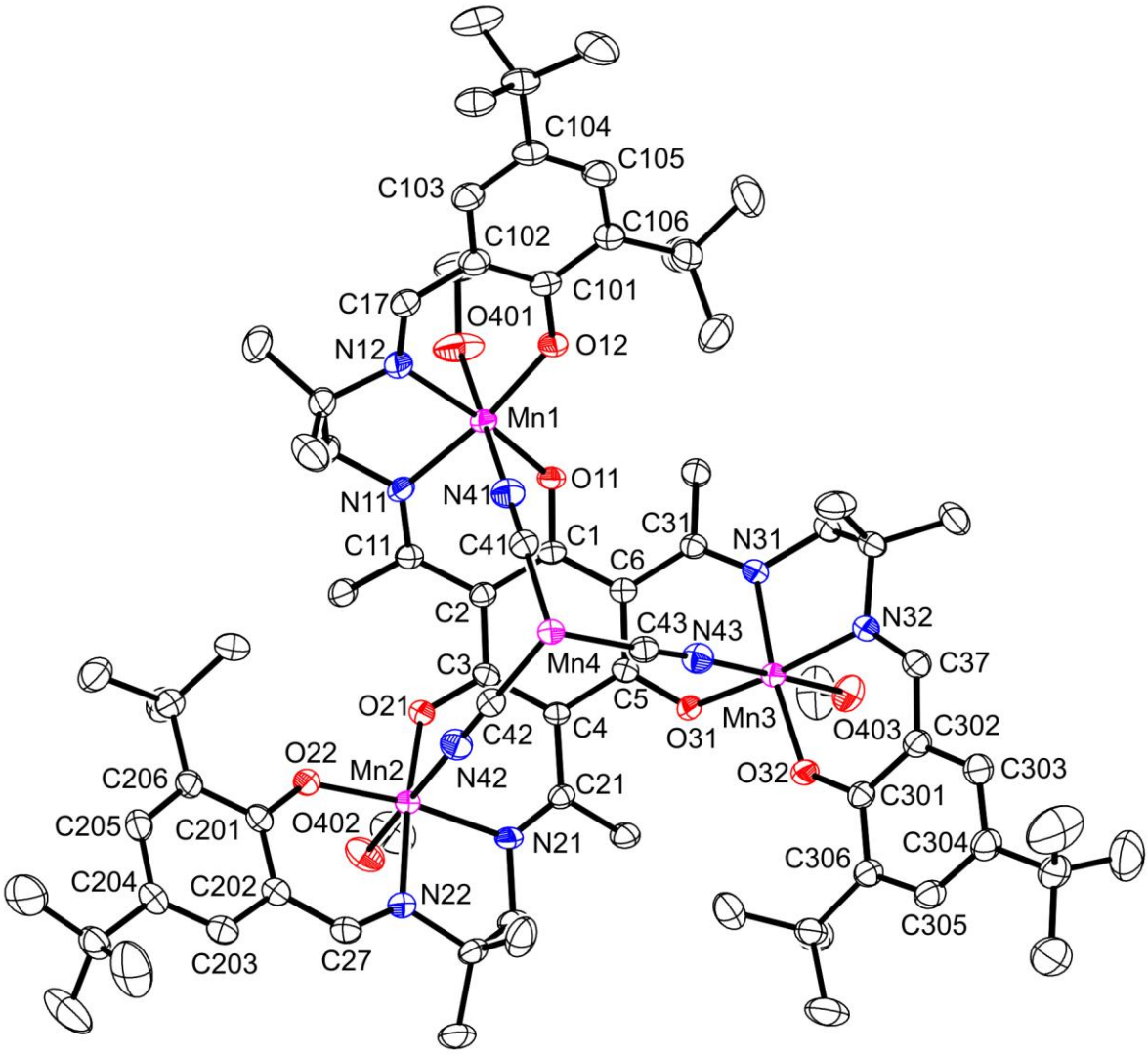

Fig. S5. Thermal ellipsoid plot of the fragment of the **$[Mn^{III}_6Mn^{III}]^{3+}$** molecule in the asymmetric unit in crystals of **5** with the numbering scheme used. Thermal ellipsoids are drawn at the 50 % probability level; hydrogen atoms are omitted for clarity.

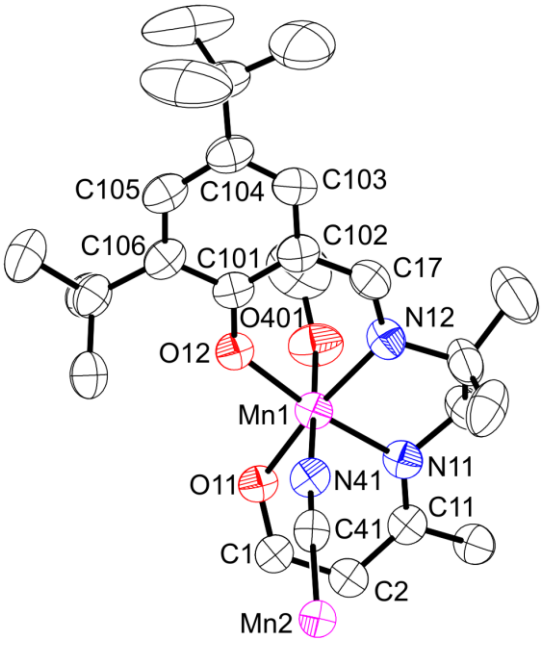

Fig. S6. Plots of the in-phase (χ'_M) and the out-of-phase (χ''_M) component of the AC susceptibility versus the temperature for **1** at zero DC field, with an AC field of 3 Oe oscillating at a frequency of 660 (orange), 1078 (blue), and 1488 Hz (black). Solid lines are a guide to the eye.

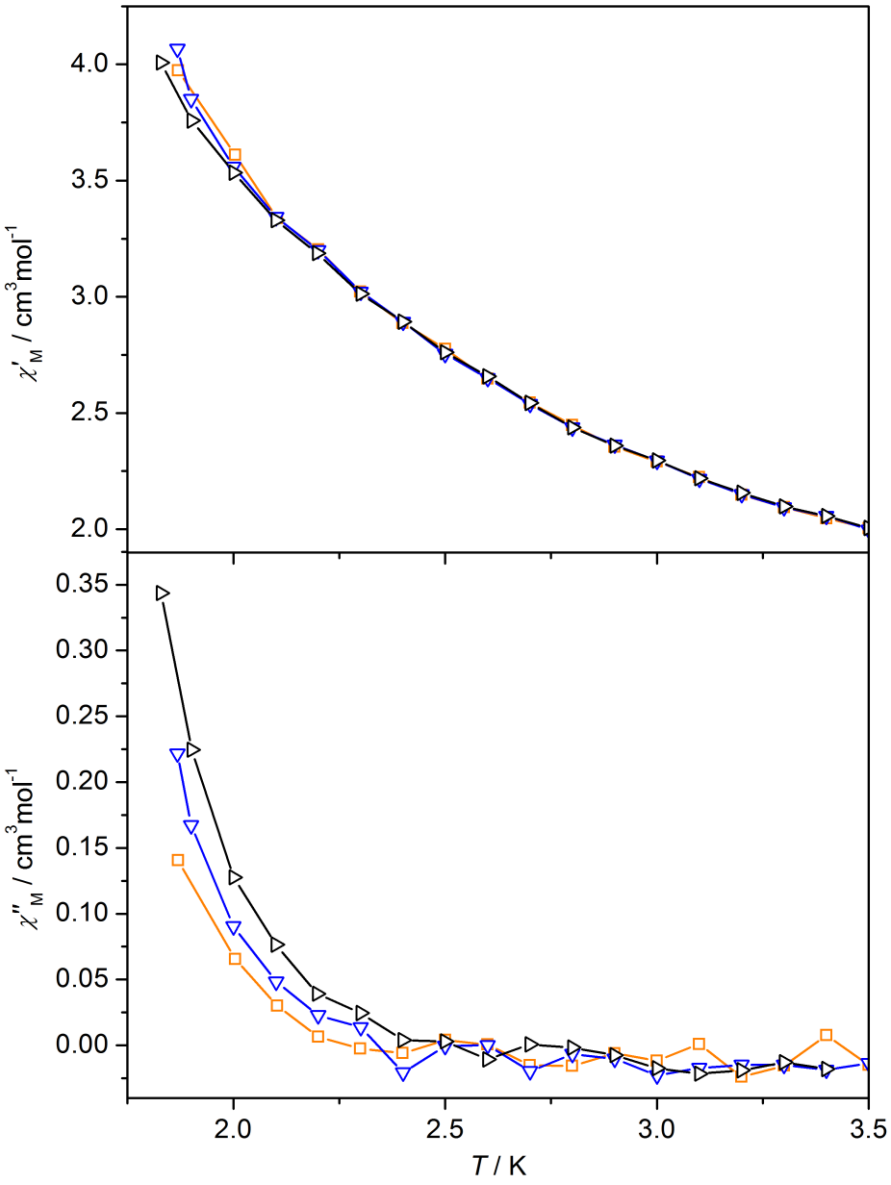

Fig. S7. Plots of the in-phase (χ'_M) and the out-of-phase (χ''_M) component of the AC susceptibility versus the temperature for **2** at zero DC field, with an AC field of 3 Oe oscillating at a frequency of 660 (orange), 1078 (blue), and 1488 Hz (black). Solid lines are a guide to the eye.

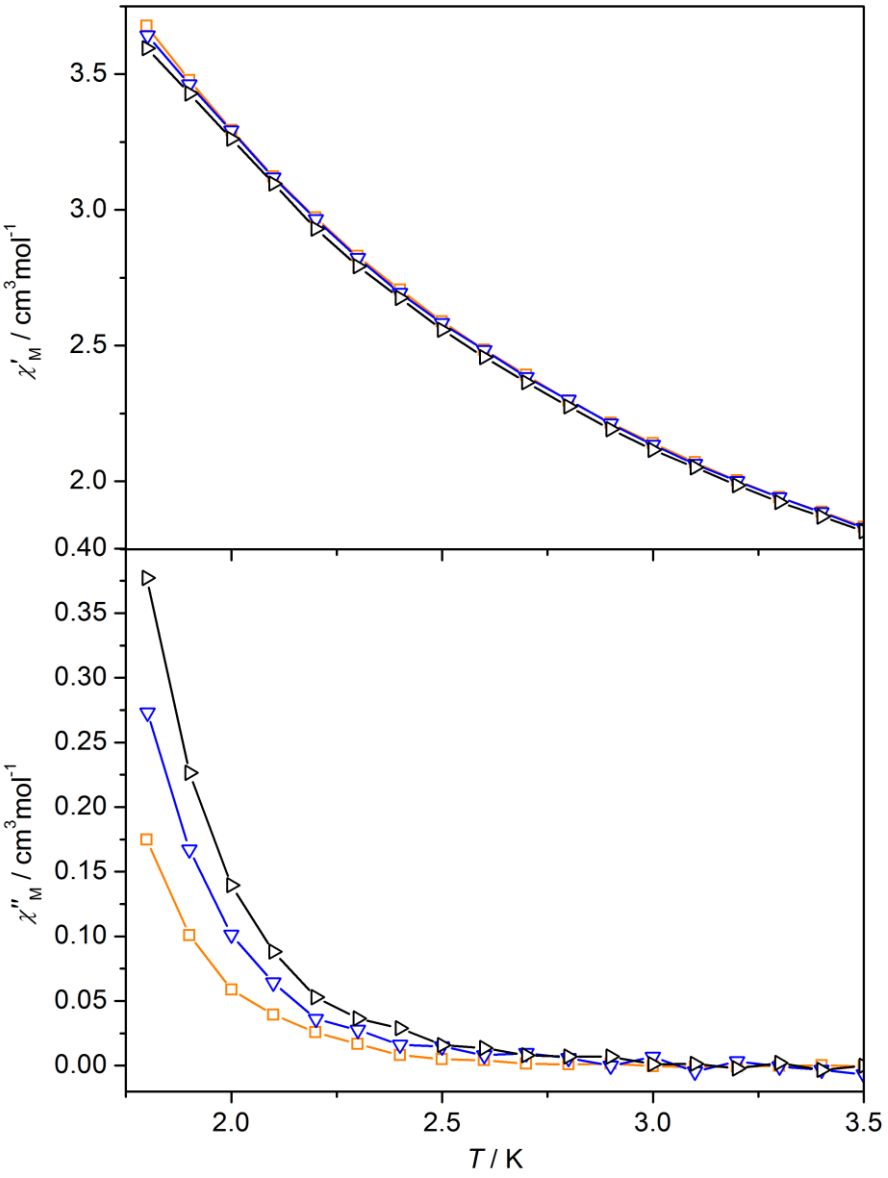

Fig. S8. Plots of the in-phase (χ'_M) and the out-of-phase (χ''_M) component of the AC susceptibility versus the temperature for **3** at zero DC field, with an AC field of 3 Oe oscillating at a frequency of 660 (orange), 1078 (blue), and 1488 Hz (black). Solid lines are a guide to the eye.

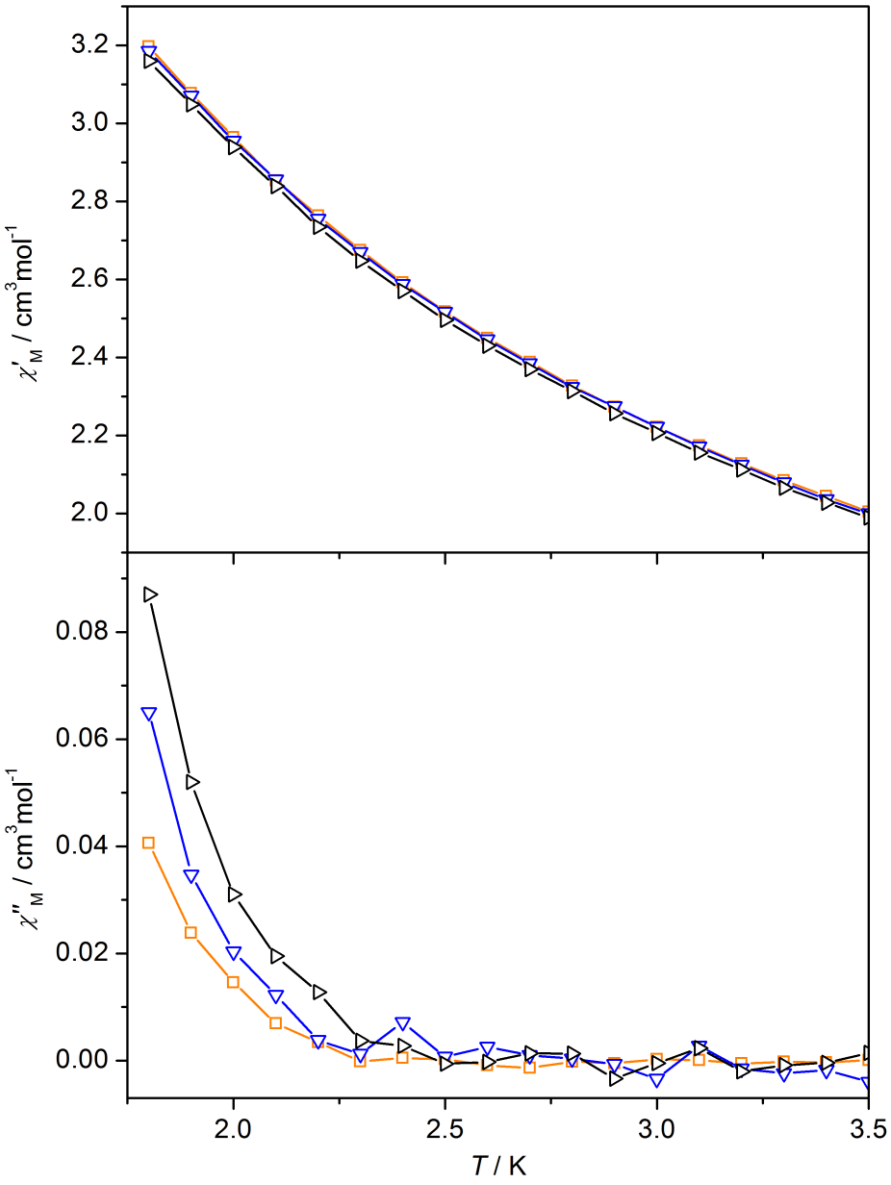

Fig. S9. Plots of the in-phase (χ'_M) and the out-of-phase (χ''_M) component of the AC susceptibility versus the temperature for **4** at zero DC field, with an AC field of 3 Oe oscillating at a frequency of 660 (orange), 1078 (blue), and 1488 Hz (black). Solid lines are a guide to the eye.

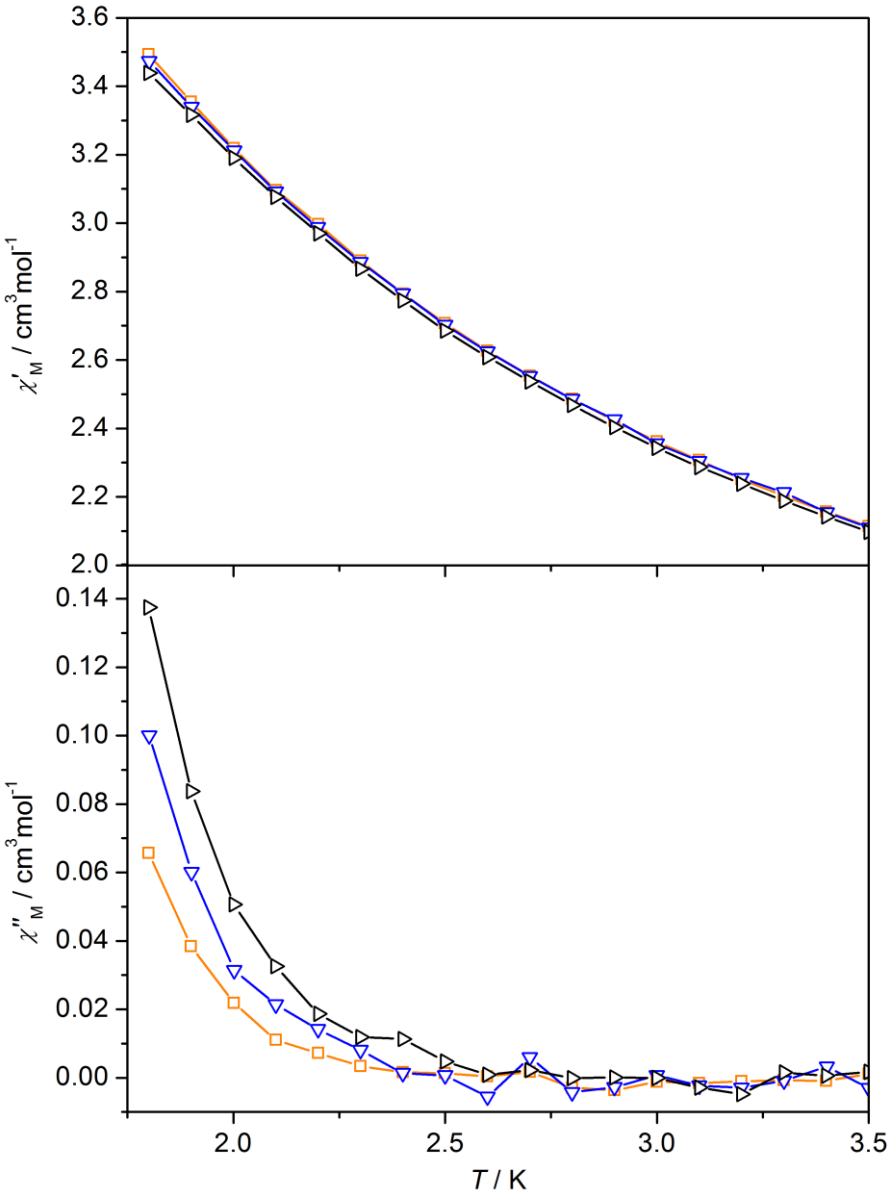

Table S1. Selected Interatomic Distances [Å] and Angles [deg] for **1**.

Mn(1)-O(11)	1.881(2)	C(202)-C(203)	1.404(4)
Mn(1)-O(12)	1.8572(19)	C(203)-C(204)	1.366(5)
Mn(1)-N(11)	1.967(2)	C(204)-C(205)	1.401(5)
Mn(1)-N(12)	1.978(2)	C(205)-C(206)	1.391(4)
Mn(1)-N(41)	2.154(2)	C(301)-C(302)	1.410(4)
Mn(2)-O(21)	1.8849(19)	C(301)-C(306)	1.425(4)
Mn(2)-O(22)	1.855(2)	C(302)-C(303)	1.407(4)
Mn(2)-N(21)	1.959(3)	C(303)-C(304)	1.379(5)
Mn(2)-N(22)	1.973(2)	C(304)-C(305)	1.407(5)
Mn(2)-N(42)	2.130(2)	C(305)-C(306)	1.381(4)
Mn(3)-O(31)	1.879(2)	Mn(1)-Mn(2)	6.6629(6)
Mn(3)-O(32)	1.860(2)	Mn(1)-Mn(3)	6.6468(7)
Mn(3)-N(31)	1.963(2)	Mn(2)-Mn(3)	6.6300(7)
Mn(3)-N(32)	1.981(2)	Mn(1)-Mn(4)	5.2203(5)
Mn(3)-N(43)	2.155(2)	Mn(2)-Mn(4)	5.1626(5)
O(11)-C(1)	1.311(3)	Mn(3)-Mn(4)	5.2312(5)
O(12)-C(101)	1.316(3)	Mn(4)-C(41)	1.995(3)
O(21)-C(3)	1.304(3)	Mn(4)-C(42)	1.982(3)
O(22)-C(201)	1.322(4)	Mn(4)-C(43)	2.002(3)
O(31)-C(5)	1.314(3)	N(41)-C(41)	1.153(4)
O(32)-C(301)	1.324(4)	N(42)-C(42)	1.151(4)
N(11)-C(11)	1.302(4)	N(43)-C(43)	1.152(4)
N(12)-C(17)	1.288(4)	Mn(5)-O(51)	1.892(2)
N(21)-C(21)	1.303(4)	Mn(5)-O(52)	1.856(2)
N(22)-C(27)	1.292(4)	Mn(5)-N(51)	1.966(3)
N(31)-C(31)	1.296(4)	Mn(5)-N(52)	1.980(2)
N(32)-C(37)	1.286(4)	Mn(5)-N(45)	2.187(3)
C(1)-C(2)	1.416(4)	Mn(6)-O(61)	1.886(2)
C(1)-C(6)	1.417(4)	Mn(6)-O(62)	1.851(2)
C(2)-C(3)	1.431(4)	Mn(6)-N(61)	1.959(3)
C(3)-C(4)	1.414(4)	Mn(6)-N(62)	1.974(3)
C(4)-C(5)	1.427(4)	Mn(6)-N(46)	2.134(3)
C(5)-C(6)	1.417(4)	Mn(7)-O(71)	1.886(2)
C(2)-C(11)	1.451(4)	Mn(7)-O(72)	1.857(2)
C(17)-C(102)	1.442(4)	Mn(7)-N(71)	1.967(3)
C(4)-C(21)	1.458(4)	Mn(7)-N(72)	1.971(3)
C(27)-C(202)	1.435(5)	Mn(7)-N(47)	2.144(3)
C(6)-C(31)	1.456(4)	O(51)-C(1A)	1.311(4)
C(37)-C(302)	1.433(4)	O(52)-C(501)	1.327(3)
C(101)-C(102)	1.413(4)	O(61)-C(3A)	1.310(4)
C(101)-C(106)	1.430(4)	O(62)-C(601)	1.323(4)
C(102)-C(103)	1.405(4)	O(71)-C(5A)	1.310(3)
C(103)-C(104)	1.368(4)	O(72)-C(701)	1.327(4)
C(104)-C(105)	1.413(4)	N(51)-C(51)	1.303(4)
C(105)-C(106)	1.377(4)	N(52)-C(57)	1.284(4)
C(201)-C(202)	1.416(4)	N(61)-C(61)	1.294(4)
C(201)-C(206)	1.418(5)	N(62)-C(67)	1.289(4)
		N(71)-C(71)	1.301(4)
		N(72)-C(77)	1.292(4)
		C(1A)-C(2A)	1.416(4)
		C(1A)-C(6A)	1.426(4)

C(2A)-C(3A)	1.425(4)
C(3A)-C(4A)	1.419(4)
C(4A)-C(5A)	1.416(4)
C(5A)-C(6A)	1.418(4)
C(2A)-C(51)	1.458(4
C(57)-C(502)	1.436(4)
C(4A)-C(61)	1.461(4)
C(67)-C(602)	1.438(5)
C(6A)-C(71)	1.459(4)
C(77)-C(702)	1.432(5)
C(501)-C(502)	1.416(4)
C(501)-C(506)	1.411(4)
C(502)-C(503)	1.407(4)
C(503)-C(504)	1.378(5)
C(504)-C(505)	1.406(5)
C(505)-C(506)	1.390(4)
C(601)-C(602)	1.410(5)
C(601)-C(606)	1.423(5)
C(602)-C(603)	1.404(5)
C(603)-C(604)	1.376(5)
C(604)-C(605)	1.405(5)
C(605)-C(606)	1.379(5)
C(701)-C(702)	1.409(4)
C(701)-C(706)	1.418(4)
C(702)-C(703)	1.408(5)
C(703)-C(704)	1.376(5)
C(704)-C(705)	1.412(4)
C(705)-C(706)	1.388(4)
Mn(5)-Mn(6)	6.7208(7)
Mn(5)-Mn(7)	6.6376(7)
Mn(6)-Mn(7)	6.6801(7)
Mn(5)-Mn(8)	5.2721(5)
Mn(6)-Mn(8)	5.1822(5)
Mn(7)-Mn(8)	5.2055(5)
Mn(8)-C(45)	1.999(3)
Mn(8)-C(46)	1.988(3)
Mn(8)-C(47)	1.993(3)
N(45)-C(45)	1.152(4)
N(46)-C(46)	1.156(4)
N(47)-C(47)	1.148(4)

O(12)-Mn(1)-O(11)	92.74(9)
O(12)-Mn(1)-N(11)	166.70(9)
O(11)-Mn(1)-N(11)	88.32(9)
O(12)-Mn(1)-N(12)	92.02(9)
O(11)-Mn(1)-N(12)	160.34(9)
N(11)-Mn(1)-N(12)	82.79(10)
O(12)-Mn(1)-N(41)	97.18(9)
O(11)-Mn(1)-N(41)	94.42(9)
N(11)-Mn(1)-N(41)	95.96(9)
N(12)-Mn(1)-N(41)	103.88(9)
O(22)-Mn(2)-O(21)	91.43(9)
O(22)-Mn(2)-N(21)	167.15(10)
O(21)-Mn(2)-N(21)	89.50(10)
O(22)-Mn(2)-N(22)	91.92(10)
O(21)-Mn(2)-N(22)	160.81(9)
N(21)-Mn(2)-N(22)	83.15(10)
O(22)-Mn(2)-N(42)	96.88(10)
O(21)-Mn(2)-N(42)	95.06(9)
N(21)-Mn(2)-N(42)	95.80(10)
N(22)-Mn(2)-N(42)	103.29(10)
O(32)-Mn(3)-O(31)	91.98(9)
O(32)-Mn(3)-N(31)	166.20(9)
O(31)-Mn(3)-N(31)	88.71(9)
O(32)-Mn(3)-N(32)	91.30(10)
O(31)-Mn(3)-N(32)	157.88(9)
N(31)-Mn(3)-N(32)	83.05(10)
O(32)-Mn(3)-N(43)	96.97(9)
O(31)-Mn(3)-N(43)	94.14(9)
N(31)-Mn(3)-N(43)	96.73(9)
N(32)-Mn(3)-N(43)	107.16(10)
Mn(4)-Mn(1)-Mn(2)	49.700(6)
Mn(4)-Mn(1)-Mn(3)	50.581(6)
Mn(4)-Mn(2)-Mn(1)	50.462(6)
Mn(4)-Mn(2)-Mn(3)	50.825(6)
Mn(4)-Mn(3)-Mn(1)	50.436(6)
Mn(4)-Mn(3)-Mn(2)	49.911(6)
Mn(3)-Mn(1)-Mn(2)	59.752(7)
Mn(3)-Mn(2)-Mn(1)	60.003(7)
Mn(2)-Mn(3)-Mn(1)	60.244(7)
C(1)-O(11)-Mn(1)	122.23(17)
C(101)-O(12)-Mn(1)	131.17(18)
C(3)-O(21)-Mn(2)	122.62(18)
C(201)-O(22)-Mn(2)	131.3(2)
C(5)-O(31)-Mn(3)	121.59(17)
C(301)-O(32)-Mn(3)	130.73(19)
C(41)-Mn(4)-C(43)	89.79(11)
C(42)-Mn(4)-C(41)	90.43(11)
C(42)-Mn(4)-C(43)	90.06(11)
Mn(1)-Mn(4)-Mn(3)	78.983(8)
Mn(2)-Mn(4)-Mn(1)	79.838(8)
Mn(2)-Mn(4)-Mn(3)	79.264(8)
C(41)-N(41)-Mn(1)	160.4(2)
C(42)-N(42)-Mn(2)	157.7(2)
C(43)-N(43)-Mn(3)	160.9(2)
N(41)-C(41)-Mn(4)	178.4(2)
N(42)-C(42)-Mn(4)	179.2(3)
N(43)-C(43)-Mn(4)	178.7(3)
O(52)-Mn(5)-O(51)	94.48(9)
O(52)-Mn(5)-N(51)	172.31(10)
O(51)-Mn(5)-N(51)	88.62(10)
O(52)-Mn(5)-N(52)	92.20(10)

O(51)-Mn(5)-N(52)	164.03(10)
N(51)-Mn(5)-N(52)	83.09(10)
O(52)-Mn(5)-N(45)	94.02(10)
O(51)-Mn(5)-N(45)	93.34(9)
N(51)-Mn(5)-N(45)	92.82(10)
N(52)-Mn(5)-N(45)	100.66(10)
O(62)-Mn(6)-O(61)	91.63(10)
O(62)-Mn(6)-N(61)	163.92(10)
O(61)-Mn(6)-N(61)	89.38(10)
O(62)-Mn(6)-N(62)	90.89(11)
O(61)-Mn(6)-N(62)	161.09(10)
N(61)-Mn(6)-N(62)	83.14(11)
O(62)-Mn(6)-N(46)	99.80(10)
O(61)-Mn(6)-N(46)	93.79(10)
N(61)-Mn(6)-N(46)	96.14(10)
N(62)-Mn(6)-N(46)	104.24(10)
O(72)-Mn(7)-O(71)	92.99(9)
O(72)-Mn(7)-N(71)	165.69(10)
O(71)-Mn(7)-N(71)	88.14(10)
O(72)-Mn(7)-N(72)	91.72(10)
O(71)-Mn(7)-N(72)	160.17(11)
N(71)-Mn(7)-N(72)	82.68(11)
O(72)-Mn(7)-N(47)	96.68(10)
O(71)-Mn(7)-N(47)	93.84(9)
N(71)-Mn(7)-N(47)	97.47(10)
N(72)-Mn(7)-N(47)	104.73(11)
Mn(8)-Mn(5)-Mn(6)	49.409(6)
Mn(8)-Mn(5)-Mn(7)	50.247(6)
Mn(8)-Mn(6)-Mn(5)	50.582(6)
Mn(8)-Mn(6)-Mn(7)	50.131(6)
Mn(8)-Mn(7)-Mn(5)	51.137(6)
Mn(8)-Mn(7)-Mn(6)	49.826(6)
Mn(7)-Mn(5)-Mn(6)	60.004(8)
Mn(7)-Mn(6)-Mn(5)	59.379(7)
Mn(5)-Mn(7)-Mn(6)	60.616(7)
C(1A)-O(51)-Mn(5)	121.80(19)
C(501)-O(52)-Mn(5)	131.8(2)
C(3A)-O(61)-Mn(6)	123.11(19)
C(601)-O(62)-Mn(6)	131.3(2)
C(5A)-O(71)-Mn(7)	122.12(18)
C(701)-O(72)-Mn(7)	131.31(19)
C(46)-Mn(8)-C(45)	90.28(11)
C(46)-Mn(8)-C(47)	91.32(12)
C(47)-Mn(8)-C(45)	88.68(12)
Mn(6)-Mn(8)-Mn(5)	80.008(8)
Mn(6)-Mn(8)-Mn(7)	80.042(8)
Mn(7)-Mn(8)-Mn(5)	78.616(8)
C(45)-N(45)-Mn(5)	162.8(2)
C(46)-N(46)-Mn(6)	158.3(3)
C(47)-N(47)-Mn(7)	160.2(2)
N(45)-C(45)-Mn(8)	178.4(3)
N(46)-C(46)-Mn(8)	178.8(3)
N(47)-C(47)-Mn(8)	179.2(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+1,-z+1 #2 -x,-y+2,-z+2

Table S2. Selected Interatomic Distances [Å] and Angles [deg] for **2**.

Mn(1)-O(11)	1.8823(16)	C(201)-C(206)	1.425(3)
Mn(1)-O(12)	1.8671(16)	C(202)-C(203)	1.408(3)
Mn(1)-N(11)	1.9641(18)	C(203)-C(204)	1.372(3)
Mn(1)-N(12)	1.9826(19)	C(204)-C(205)	1.403(3)
Mn(1)-N(41)	2.1412(19)	C(205)-C(206)	1.382(3)
Mn(2)-O(21)	1.8852(15)	C(301)-C(302)	1.419(3)
Mn(2)-O(22)	1.8602(16)	C(301)-C(306)	1.424(3)
Mn(2)-N(21)	1.9628(19)	C(302)-C(303)	1.406(3)
Mn(2)-N(22)	1.9817(19)	C(303)-C(304)	1.371(4)
Mn(2)-N(42)	2.137(2)	C(304)-C(305)	1.401(4)
Mn(3)-O(31)	1.8980(15)	C(305)-C(306)	1.383(4)
Mn(3)-O(32)	1.8723(16)	Mn(1)-Mn(2)	6.6368(5)
Mn(3)-N(31)	1.9711(19)	Mn(1)-Mn(3)	6.6604(5)
Mn(3)-N(32)	1.9848(18)	Mn(2)-Mn(3)	6.6891(5)
Mn(3)-N(43)	2.230(2)	Mn(1)-Mn(4)	5.1923(4)
Mn(3)-O(403)	2.3139(18)	Mn(2)-Mn(4)	5.1882(3)
O(11)-C(1)	1.311(3)	Mn(3)-Mn(4)	5.3149(4)
O(12)-C(101)	1.319(3)	Mn(4)-C(41)#1	1.987(2)
O(21)-C(3)	1.317(3)	Mn(4)-C(42)	1.988(2)
O(22)-C(201)	1.321(3)	Mn(4)-C(43)	1.998(2)
O(31)-C(5)	1.312(3)	N(41)-C(41)#1	1.152(3)
O(32)-C(301)	1.313(3)	N(42)-C(42)	1.152(3)
N(11)-C(11)	1.303(3)	N(43)-C(43)	1.151(3)
N(12)-C(17)	1.290(3)	Mn(5)-O(51)	1.8881(16)
N(21)-C(21)	1.305(3)	Mn(5)-O(52)	1.8674(15)
N(22)-C(27)	1.289(3)	Mn(5)-N(51)	1.9653(18)
N(31)-C(31)	1.302(3)	Mn(5)-N(52)	1.9921(19)
N(32)-C(37)	1.282(3)	Mn(5)-N(85)	2.2417(19)
C(1)-C(2)	1.419(3)	Mn(5)-O(805)	2.3886(19)
C(1)-C(6)	1.425(3)	Mn(6)-O(61)	1.8943(15)
C(2)-C(3)	1.424(3)	Mn(6)-O(62)	1.8599(16)
C(3)-C(4)	1.416(3)	Mn(6)-N(61)	1.9628(19)
C(4)-C(5)	1.432(3)	Mn(6)-N(62)	1.9903(19)
C(5)-C(6)	1.409(3)	Mn(6)-N(86)	2.2009(19)
C(2)-C(11)	1.460(3)	Mn(6)-O(806)	2.394(2)
C(17)-C(102)	1.435(3)	Mn(7)-O(71)	1.8860(15)
C(4)-C(21)	1.455(3)	Mn(7)-O(72)	1.8650(15)
C(27)-C(202)	1.433(3)	Mn(7)-N(71)	1.9644(18)
C(6)-C(31)	1.462(3)	Mn(7)-N(72)	1.9845(18)
C(37)-C(302)	1.438(3)	Mn(7)-N(87)	2.214(2)
C(101)-C(102)	1.417(3)	Mn(7)-O(807)	2.496(2)
C(101)-C(106)	1.428(3)	O(51)-C(45)	1.308(3)
C(102)-C(103)	1.410(3)	O(52)-C(501)	1.309(3)
C(103)-C(104)	1.371(4)	O(61)-C(47)	1.309(3)
C(104)-C(105)	1.415(3)	O(62)-C(601)	1.315(3)
C(105)-C(106)	1.377(3)	O(71)-C(49)	1.316(3)
C(201)-C(202)	1.413(3)	O(72)-C(701)	1.319(3)
		N(51)-C(51)	1.298(3)
		N(52)-C(57)	1.284(3)
		N(61)-C(61)	1.301(3)
		N(62)-C(67)	1.289(3)

N(71)-C(71)	1.300(3)
N(72)-C(77)	1.288(3)
C(45)-C(46)	1.417(3)
C(45)-C(50)	1.422(3)
C(46)-C(47)	1.431(3)
C(47)-C(48)	1.419(3)
C(48)-C(49)	1.419(3)
C(49)-C(50)	1.413(3)
C(46)-C(51)	1.461(3)
C(57)-C(502)	1.447(3)
C(48)-C(61)	1.462(3)
C(67)-C(602)	1.439(3)
C(50)-C(71)	1.464(3)
C(77)-C(702)	1.437(3)
C(501)-C(502)	1.418(3)
C(501)-C(506)	1.433(3)
C(502)-C(503)	1.408(3)
C(503)-C(504)	1.374(3)
C(504)-C(505)	1.407(3)
C(505)-C(506)	1.382(3)
C(601)-C(602)	1.416(3)
C(601)-C(606)	1.423(3)
C(602)-C(603)	1.411(3)
C(603)-C(604)	1.377(4)
C(604)-C(605)	1.405(4)
C(605)-C(606)	1.378(3)
C(701)-C(702)	1.413(3)
C(701)-C(706)	1.426(3)
C(702)-C(703)	1.414(3)
C(703)-C(704)	1.372(3)
C(704)-C(705)	1.408(3)
C(705)-C(706)	1.387(3)
Mn(5)-Mn(6)	6.6856(5)
Mn(5)-Mn(7)	6.6867(5)
Mn(6)-Mn(7)	6.7051(5)
Mn(5)-Mn(8)	5.3390(3)
Mn(6)-Mn(8)	5.2756(4)
Mn(7)-Mn(8)	5.2974(4)
Mn(8)-C(85)	2.017(2)
Mn(8)-C(86)	1.995(2)
Mn(8)-C(87)	2.003(2)
N(85)-C(85)	1.149(3)
N(86)-C(86)	1.155(3)
N(87)-C(87)	1.154(3)

O(12)-Mn(1)-O(11)	94.16(7)
O(12)-Mn(1)-N(11)	169.46(7)
O(11)-Mn(1)-N(11)	88.03(7)
O(12)-Mn(1)-N(12)	91.50(7)
O(11)-Mn(1)-N(12)	158.86(8)
N(11)-Mn(1)-N(12)	82.95(8)
O(12)-Mn(1)-N(41)	94.53(7)
O(11)-Mn(1)-N(41)	96.10(7)
N(11)-Mn(1)-N(41)	95.48(8)
N(12)-Mn(1)-N(41)	103.74(8)
O(22)-Mn(2)-O(21)	92.60(7)
O(22)-Mn(2)-N(21)	163.64(8)
O(21)-Mn(2)-N(21)	87.92(7)
O(22)-Mn(2)-N(22)	91.24(7)
O(21)-Mn(2)-N(22)	158.77(7)
N(21)-Mn(2)-N(22)	82.65(8)
O(22)-Mn(2)-N(42)	98.24(8)
O(21)-Mn(2)-N(42)	95.44(7)
N(21)-Mn(2)-N(42)	97.98(8)
N(22)-Mn(2)-N(42)	104.65(8)
O(32)-Mn(3)-O(31)	94.90(7)
O(32)-Mn(3)-N(31)	174.90(7)
O(31)-Mn(3)-N(31)	89.02(7)
O(32)-Mn(3)-N(32)	92.91(7)
O(31)-Mn(3)-N(32)	168.05(7)
N(31)-Mn(3)-N(32)	82.72(8)
O(32)-Mn(3)-N(43)	91.14(8)
O(31)-Mn(3)-N(43)	91.67(7)
N(31)-Mn(3)-N(43)	92.02(8)
N(32)-Mn(3)-N(43)	97.21(8)
O(32)-Mn(3)-O(403)	88.56(7)
O(31)-Mn(3)-O(403)	88.17(7)
N(31)-Mn(3)-O(403)	88.29(8)
N(32)-Mn(3)-O(403)	82.98(7)
N(43)-Mn(3)-O(403)	179.65(8)
Mn(4)-Mn(1)-Mn(2)	50.229(4)
Mn(4)-Mn(1)-Mn(3)	51.482(5)
Mn(4)-Mn(2)-Mn(1)	50.284(4)
Mn(4)-Mn(2)-Mn(3)	51.283(5)
Mn(4)-Mn(3)-Mn(1)	49.852(4)
Mn(4)-Mn(3)-Mn(2)	49.609(4)
Mn(2)-Mn(1)-Mn(3)	60.403(6)
Mn(1)-Mn(2)-Mn(3)	59.973(5)
Mn(1)-Mn(3)-Mn(2)	59.624(5)
C(1)-O(11)-Mn(1)	121.63(13)
C(101)-O(12)-Mn(1)	131.83(14)
C(3)-O(21)-Mn(2)	121.96(14)
C(201)-O(22)-Mn(2)	131.96(15)
C(5)-O(31)-Mn(3)	122.36(14)
C(301)-O(32)-Mn(3)	130.64(15)
C(41)#1-Mn(4)-C(42)	89.62(9)
C(41)#1-Mn(4)-C(43)	89.35(9)
C(42)-Mn(4)-C(43)	89.73(9)
Mn(1)-Mn(4)-Mn(3)	78.666(6)
Mn(2)-Mn(4)-Mn(1)	79.487(5)
Mn(2)-Mn(4)-Mn(3)	79.108(6)
C(41)#1-N(41)-Mn(1)	160.39(19)

C(42)-N(42)-Mn(2)	159.84(18)
C(43)-N(43)-Mn(3)	163.19(19)
N(41)#1-C(41)-Mn(4)	177.3(2)
N(42)-C(42)-Mn(4)	178.0(2)
N(43)-C(43)-Mn(4)	178.1(2)
O(52)-Mn(5)-O(51)	94.23(7)
O(52)-Mn(5)-N(51)	173.32(7)
O(51)-Mn(5)-N(51)	88.79(7)
O(52)-Mn(5)-N(52)	92.07(7)
O(51)-Mn(5)-N(52)	163.84(7)
N(51)-Mn(5)-N(52)	83.51(8)
O(52)-Mn(5)-N(85)	92.03(7)
O(51)-Mn(5)-N(85)	92.66(7)
N(51)-Mn(5)-N(85)	93.79(7)
N(52)-Mn(5)-N(85)	101.98(8)
O(52)-Mn(5)-O(805)	89.37(7)
O(51)-Mn(5)-O(805)	83.84(8)
N(51)-Mn(5)-O(805)	85.02(7)
N(52)-Mn(5)-O(805)	81.36(8)
N(85)-Mn(5)-O(805)	176.32(8)
O(62)-Mn(6)-O(61)	95.10(7)
O(62)-Mn(6)-N(61)	174.03(8)
O(61)-Mn(6)-N(61)	88.50(7)
O(62)-Mn(6)-N(62)	91.80(7)
O(61)-Mn(6)-N(62)	163.61(7)
N(61)-Mn(6)-N(62)	83.52(8)
O(62)-Mn(6)-N(86)	91.79(8)
O(61)-Mn(6)-N(86)	94.23(7)
N(61)-Mn(6)-N(86)	92.69(8)
N(62)-Mn(6)-N(86)	100.40(8)
O(62)-Mn(6)-O(806)	90.42(8)
O(61)-Mn(6)-O(806)	83.70(7)
N(61)-Mn(6)-O(806)	85.24(8)
N(62)-Mn(6)-O(806)	81.40(8)
N(86)-Mn(6)-O(806)	177.10(8)
O(72)-Mn(7)-O(71)	93.67(7)
O(72)-Mn(7)-N(71)	171.37(8)
O(71)-Mn(7)-N(71)	89.38(7)
O(72)-Mn(7)-N(72)	91.91(7)
O(71)-Mn(7)-N(72)	164.43(7)
N(71)-Mn(7)-N(72)	83.16(7)
O(72)-Mn(7)-N(87)	93.88(7)
O(71)-Mn(7)-N(87)	92.97(7)
N(71)-Mn(7)-N(87)	94.01(8)
N(72)-Mn(7)-N(87)	101.15(8)
O(72)-Mn(7)-O(807)	90.92(7)
O(71)-Mn(7)-O(807)	83.44(7)
N(71)-Mn(7)-O(807)	81.40(7)
N(72)-Mn(7)-O(807)	81.95(7)
N(87)-Mn(7)-O(807)	174.18(7)
Mn(8)-Mn(5)-Mn(6)	50.540(5)
Mn(8)-Mn(5)-Mn(7)	50.772(4)
Mn(8)-Mn(6)-Mn(5)	51.384(4)
Mn(8)-Mn(6)-Mn(7)	50.786(4)
Mn(8)-Mn(7)-Mn(5)	51.326(4)
Mn(8)-Mn(7)-Mn(6)	50.497(4)
Mn(6)-Mn(5)-Mn(7)	60.188(6)
Mn(5)-Mn(6)-Mn(7)	59.914(5)
Mn(5)-Mn(7)-Mn(6)	59.898(5)
C(45)-O(51)-Mn(5)	122.55(14)
C(501)-O(52)-Mn(5)	131.48(14)
C(47)-O(61)-Mn(6)	122.30(13)
C(601)-O(62)-Mn(6)	131.94(15)
C(49)-O(71)-Mn(7)	122.76(14)
C(701)-O(72)-Mn(7)	131.33(14)
C(86)-Mn(8)-C(85)	88.41(9)
C(86)-Mn(8)-C(87)	88.59(9)
C(87)-Mn(8)-C(85)	88.44(9)
Mn(6)-Mn(8)-Mn(5)	78.076(6)
Mn(6)-Mn(8)-Mn(7)	78.717(6)
Mn(7)-Mn(8)-Mn(5)	77.902(6)
C(85)-N(85)-Mn(5)	163.14(19)
C(86)-N(86)-Mn(6)	162.09(18)
C(87)-N(87)-Mn(7)	162.41(18)
N(85)-C(85)-Mn(8)	177.3(2)
N(86)-C(86)-Mn(8)	177.2(2)
N(87)-C(87)-Mn(8)	177.31(19)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x,-y+2,-z+2

Table S3. Selected Interatomic Distances [Å] and Angles [deg] for **3**.

Mn(1)-O(11)	1.894(2)	C(105)-C(106)	1.395(5)
Mn(1)-O(12)	1.876(2)	C(201)-C(202)	1.421(5)
Mn(1)-N(11)	1.987(3)	C(201)-C(206)	1.424(5)
Mn(1)-N(12)	1.985(3)	C(202)-C(203)	1.404(5)
Mn(1)-N(41)	2.207(3)	C(203)-C(204)	1.382(5)
Mn(1)-O(401)	2.350(3)	C(204)-C(205)	1.406(5)
Mn(2)-O(21)	1.897(2)	C(205)-C(206)	1.390(5)
Mn(2)-O(22)	1.873(2)	C(301)-C(302)	1.410(5)
Mn(2)-N(21)	1.983(3)	C(301)-C(306)	1.426(5)
Mn(2)-N(22)	1.981(3)	C(302)-C(303)	1.421(5)
Mn(2)-N(42)	2.213(3)	C(303)-C(304)	1.370(5)
Mn(2)-O(402)	2.350(3)	C(304)-C(305)	1.400(5)
Mn(3)-O(31)	1.887(2)	C(305)-C(306)	1.396(5)
Mn(3)-O(32)	1.874(2)	Mn(1)-Mn(2)	6.8588(7)
Mn(3)-N(31)	1.981(3)	Mn(1)-Mn(3)	6.7944(7)
Mn(3)-N(32)	1.979(3)	Mn(2)-Mn(3)	6.8240(7)
Mn(3)-N(43)	2.200(3)	Mn(1)-Mn(4)	5.2945(5)
Mn(3)-O(403)	2.400(3)	Mn(2)-Mn(4)	5.2836(5)
O(11)-C(1)	1.305(4)	Mn(3)-Mn(4)	5.2679(5)
O(12)-C(101)	1.327(4)	Mn(4)-C(41)	1.993(3)
O(21)-C(3)	1.308(4)	Mn(4)-C(42)	1.992(3)
O(22)-C(201)	1.315(4)	Mn(4)-C(43)	1.988(3)
O(31)-C(5)	1.316(4)	N(41)-C(41)	1.148(4)
O(32)-C(301)	1.327(4)	N(42)-C(42)	1.148(4)
N(11)-C(11)	1.301(4)	N(43)-C(43)	1.148(4)
N(12)-C(17)	1.282(5)		
N(21)-C(21)	1.293(4)	O(12)-Mn(1)-O(11)	96.07(10)
N(22)-C(27)	1.282(5)	O(12)-Mn(1)-N(12)	91.96(11)
N(31)-C(31)	1.304(4)	O(11)-Mn(1)-N(12)	169.25(11)
N(32)-C(37)	1.295(4)	O(12)-Mn(1)-N(11)	171.70(11)
C(1)-C(2)	1.423(4)	O(11)-Mn(1)-N(11)	88.16(10)
C(1)-C(6)	1.436(4)	N(12)-Mn(1)-N(11)	83.01(12)
C(2)-C(3)	1.426(4)	O(12)-Mn(1)-N(41)	95.26(11)
C(3)-C(4)	1.423(4)	O(11)-Mn(1)-N(41)	90.34(11)
C(4)-C(5)	1.418(4)	N(12)-Mn(1)-N(41)	96.04(12)
C(5)-C(6)	1.414(4)	N(11)-Mn(1)-N(41)	91.85(12)
C(2)-C(11)	1.472(4)	O(12)-Mn(1)-O(401)	86.81(11)
C(17)-C(102)	1.437(5)	O(11)-Mn(1)-O(401)	87.76(10)
C(4)-C(21)	1.464(4)	N(12)-Mn(1)-O(401)	85.56(12)
C(27)-C(202)	1.436(5)	N(11)-Mn(1)-O(401)	86.22(11)
C(6)-C(31)	1.458(5)	N(41)-Mn(1)-O(401)	177.33(11)
C(37)-C(302)	1.435(5)	O(22)-Mn(2)-O(21)	96.12(10)
C(101)-C(102)	1.418(5)	O(22)-Mn(2)-N(22)	91.27(11)
C(101)-C(106)	1.430(5)	O(21)-Mn(2)-N(22)	169.94(11)
C(102)-C(103)	1.409(5)	O(22)-Mn(2)-N(21)	172.03(11)
C(103)-C(104)	1.369(6)	O(21)-Mn(2)-N(21)	89.06(11)
C(104)-C(105)	1.399(6)	N(22)-Mn(2)-N(21)	82.90(12)
		O(22)-Mn(2)-N(42)	94.83(11)
		O(21)-Mn(2)-N(42)	89.22(11)
		N(22)-Mn(2)-N(42)	96.97(12)
		N(21)-Mn(2)-N(42)	91.28(11)

O(22)-Mn(2)-O(402)	89.84(11)
O(21)-Mn(2)-O(402)	84.72(10)
N(22)-Mn(2)-O(402)	88.50(11)
N(21)-Mn(2)-O(402)	84.60(11)
N(42)-Mn(2)-O(402)	172.72(11)
O(32)-Mn(3)-O(31)	96.10(10)
O(32)-Mn(3)-N(32)	91.77(11)
O(31)-Mn(3)-N(32)	168.52(11)
O(32)-Mn(3)-N(31)	170.68(11)
O(31)-Mn(3)-N(31)	87.97(11)
N(32)-Mn(3)-N(31)	83.06(11)
O(32)-Mn(3)-N(43)	94.47(11)
O(31)-Mn(3)-N(43)	90.06(11)
N(32)-Mn(3)-N(43)	97.66(12)
N(31)-Mn(3)-N(43)	93.90(11)
O(32)-Mn(3)-O(403)	85.81(11)
O(31)-Mn(3)-O(403)	86.39(10)
N(32)-Mn(3)-O(403)	85.86(11)
N(31)-Mn(3)-O(403)	86.09(11)
N(43)-Mn(3)-O(403)	176.46(11)
Mn(4)-Mn(1)-Mn(2)	49.510(6)
Mn(4)-Mn(1)-Mn(3)	49.793(6)
Mn(4)-Mn(2)-Mn(1)	49.648(6)
Mn(4)-Mn(2)-Mn(3)	49.604(6)
Mn(4)-Mn(3)-Mn(1)	50.136(6)
Mn(4)-Mn(3)-Mn(2)	49.805(6)
Mn(3)-Mn(1)-Mn(2)	59.973(7)
Mn(3)-Mn(2)-Mn(1)	59.546(7)
Mn(1)-Mn(3)-Mn(2)	60.482(7)
C(1)-O(11)-Mn(1)	123.7(2)
C(101)-O(12)-Mn(1)	130.9(2)
C(3)-O(21)-Mn(2)	124.99(19)
C(201)-O(22)-Mn(2)	131.3(2)
C(5)-O(31)-Mn(3)	124.52(19)
C(301)-O(32)-Mn(3)	131.3(2)
C(42)-Mn(4)-C(41)	91.32(13)
C(43)-Mn(4)-C(41)	90.04(13)
C(43)-Mn(4)-C(42)	91.47(13)
Mn(2)-Mn(4)-Mn(1)	80.841(8)
Mn(3)-Mn(4)-Mn(1)	80.071(7)
Mn(3)-Mn(4)-Mn(2)	80.591(8)
C(41)-N(41)-Mn(1)	163.3(3)
C(42)-N(42)-Mn(2)	160.5(3)
C(43)-N(43)-Mn(3)	161.2(3)
N(41)-C(41)-Mn(4)	179.6(3)
N(42)-C(42)-Mn(4)	178.8(3)
N(43)-C(43)-Mn(4)	178.7(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+2

Table S4. Selected Interatomic Distances [Å] and Angles [deg] for **4**.

Mn(1)-O(11)	1.8890(18)	C(105)-C(106)	1.396(4)
Mn(1)-O(12)	1.8760(19)	C(201)-C(202)	1.421(4)
Mn(1)-N(11)	1.985(2)	C(201)-C(206)	1.423(4)
Mn(1)-N(12)	1.981(2)	C(202)-C(203)	1.415(4)
Mn(1)-N(41)	2.199(2)	C(203)-C(204)	1.371(4)
Mn(1)-O(401)	2.366(2)	C(204)-C(205)	1.406(4)
Mn(2)-O(21)	1.8948(18)	C(205)-C(206)	1.389(4)
Mn(2)-O(22)	1.8721(18)	C(301)-C(302)	1.421(4)
Mn(2)-N(21)	1.979(2)	C(301)-C(306)	1.423(4)
Mn(2)-N(22)	1.982(2)	C(302)-C(303)	1.411(4)
Mn(2)-N(42)	2.204(2)	C(303)-C(304)	1.375(4)
Mn(2)-O(402)	2.338(2)	C(304)-C(305)	1.401(4)
Mn(3)-O(31)	1.8905(18)	C(305)-C(306)	1.391(4)
Mn(3)-O(32)	1.8751(18)	Mn(1)-Mn(2)	6.8535(6)
Mn(3)-N(31)	1.982(2)	Mn(1)-Mn(3)	6.7926(6)
Mn(3)-N(32)	1.980(2)	Mn(2)-Mn(3)	6.8217(6)
Mn(3)-N(43)	2.205(2)	Mn(1)-Mn(4)	5.2860(5)
Mn(3)-O(403)	2.380(2)	Mn(2)-Mn(4)	5.2758(4)
O(11)-C(1)	1.312(3)	Mn(3)-Mn(4)	5.2847(4)
O(12)-C(101)	1.325(3)	Mn(4)-C(41)	1.991(3)
O(21)-C(3)	1.314(3)	Mn(4)-C(42)	1.991(3)
O(22)-C(201)	1.318(3)	Mn(4)-C(43)	1.995(3)
O(31)-C(5)	1.309(3)	N(41)-C(41)	1.151(4)
O(32)-C(301)	1.318(3)	N(42)-C(42)	1.149(4)
N(11)-C(11)	1.307(3)	N(43)-C(43)	1.152(3)
N(12)-C(17)	1.289(4)		
N(21)-C(21)	1.305(3)	O(12)-Mn(1)-O(11)	96.10(8)
N(22)-C(27)	1.287(4)	O(12)-Mn(1)-N(12)	91.88(9)
N(31)-C(31)	1.300(3)	O(11)-Mn(1)-N(12)	169.22(9)
N(32)-C(37)	1.289(4)	O(12)-Mn(1)-N(11)	171.48(9)
C(1)-C(6)	1.426(3)	O(11)-Mn(1)-N(11)	88.20(8)
C(1)-C(2)	1.426(3)	N(12)-Mn(1)-N(11)	82.99(9)
C(2)-C(3)	1.426(3)	O(12)-Mn(1)-N(41)	95.29(9)
C(3)-C(4)	1.418(3)	O(11)-Mn(1)-N(41)	90.75(9)
C(4)-C(5)	1.430(3)	N(12)-Mn(1)-N(41)	95.74(9)
C(5)-C(6)	1.415(3)	N(11)-Mn(1)-N(41)	92.00(9)
C(2)-C(11)	1.459(3)	O(12)-Mn(1)-O(401)	86.12(9)
C(17)-C(102)	1.436(4)	O(11)-Mn(1)-O(401)	87.02(9)
C(4)-C(21)	1.460(3)	N(12)-Mn(1)-O(401)	86.29(10)
C(27)-C(202)	1.428(4)	N(11)-Mn(1)-O(401)	86.76(9)
C(6)-C(31)	1.466(3)	N(41)-Mn(1)-O(401)	177.49(9)
C(37)-C(302)	1.441(4)	O(22)-Mn(2)-O(21)	95.90(8)
C(101)-C(102)	1.418(4)	O(22)-Mn(2)-N(21)	171.77(9)
C(101)-C(106)	1.423(4)	O(21)-Mn(2)-N(21)	89.22(8)
C(102)-C(103)	1.409(4)	O(22)-Mn(2)-N(22)	91.29(9)
C(103)-C(104)	1.375(4)	O(21)-Mn(2)-N(22)	170.05(9)
C(104)-C(105)	1.394(4)	N(21)-Mn(2)-N(22)	82.90(9)
		O(22)-Mn(2)-N(42)	94.62(9)
		O(21)-Mn(2)-N(42)	89.53(9)
		N(21)-Mn(2)-N(42)	91.86(9)
		N(22)-Mn(2)-N(42)	96.75(10)

O(22)-Mn(2)-O(402)	89.25(9)
O(21)-Mn(2)-O(402)	84.63(8)
N(21)-Mn(2)-O(402)	84.81(9)
N(22)-Mn(2)-O(402)	88.61(9)
N(42)-Mn(2)-O(402)	173.31(9)
O(32)-Mn(3)-O(31)	96.13(8)
O(32)-Mn(3)-N(32)	91.54(9)
O(31)-Mn(3)-N(32)	168.65(9)
O(32)-Mn(3)-N(31)	171.05(9)
O(31)-Mn(3)-N(31)	88.02(8)
N(32)-Mn(3)-N(31)	83.27(9)
O(32)-Mn(3)-N(43)	94.58(9)
O(31)-Mn(3)-N(43)	89.81(8)
N(32)-Mn(3)-N(43)	97.93(9)
N(31)-Mn(3)-N(43)	93.36(9)
O(32)-Mn(3)-O(403)	86.72(8)
O(31)-Mn(3)-O(403)	86.94(8)
N(32)-Mn(3)-O(403)	85.15(9)
N(31)-Mn(3)-O(403)	85.58(8)
N(43)-Mn(3)-O(403)	176.61(8)
Mn(4)-Mn(1)-Mn(2)	49.477(5)
Mn(4)-Mn(1)-Mn(3)	50.006(5)
Mn(4)-Mn(2)-Mn(1)	49.607(6)
Mn(4)-Mn(2)-Mn(3)	49.819(5)
Mn(4)-Mn(3)-Mn(1)	50.023(5)
Mn(4)-Mn(3)-Mn(2)	49.705(6)
Mn(3)-Mn(1)-Mn(2)	59.985(6)
Mn(3)-Mn(2)-Mn(1)	59.564(6)
Mn(1)-Mn(3)-Mn(2)	60.450(6)
C(1)-O(11)-Mn(1)	123.60(16)
C(101)-O(12)-Mn(1)	131.12(17)
C(3)-O(21)-Mn(2)	124.67(16)
C(201)-O(22)-Mn(2)	131.28(17)
C(5)-O(31)-Mn(3)	124.53(15)
C(301)-O(32)-Mn(3)	131.63(17)
C(41)-Mn(4)-C(43)	89.99(11)
C(42)-Mn(4)-C(41)	91.54(11)
C(42)-Mn(4)-C(43)	91.43(11)
Mn(2)-Mn(4)-Mn(1)	80.917(7)
Mn(2)-Mn(4)-Mn(3)	80.477(6)
Mn(3)-Mn(4)-Mn(1)	79.970(6)
C(41)-N(41)-Mn(1)	163.0(2)
C(42)-N(42)-Mn(2)	160.5(2)
C(43)-N(43)-Mn(3)	161.5(2)
N(41)-C(41)-Mn(4)	179.8(3)
N(42)-C(42)-Mn(4)	178.5(3)
N(43)-C(43)-Mn(4)	178.8(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+2 #2 -x+1,-y,-z+2

Table S5. Selected Interatomic Distances [Å] and Angles [deg] for **5**.

Mn(1)-O(11)	1.894(2)
Mn(1)-O(12)	1.887(2)
Mn(1)-N(11)	1.975(3)
Mn(1)-N(12)	1.990(3)
Mn(1)-N(41)	2.169(3)
Mn(1)-O(401)	2.302(3)
O(11)-C(1)	1.307(4)
O(12)-C(101)	1.320(4)
N(11)-C(11)	1.296(4)
N(12)-C(17)	1.276(5)
C(1)-C(2)	1.428(5)
C(1)-C(2)#2	1.416(5)
C(2)-C(11)	1.451(5)
C(17)-C(102)	1.431(5)
C(101)-C(102)	1.416(5)
C(101)-C(106)	1.422(5)
C(102)-C(103)	1.400(5)
C(103)-C(104)	1.362(6)
C(104)-C(105)	1.428(6)
C(105)-C(106)	1.380(5)
Mn(1)-Mn(1)#1	6.8508(9)
Mn(1)-Mn(2)	5.1997(5)
Mn(2)-C(41)	1.978(4)
N(41)-C(41)	1.147(4)
O(12)-Mn(1)-O(11)	97.42(10)
O(12)-Mn(1)-N(11)	171.49(11)
O(11)-Mn(1)-N(11)	87.62(11)
O(12)-Mn(1)-N(12)	91.36(11)
O(11)-Mn(1)-N(12)	170.28(11)
N(11)-Mn(1)-N(12)	83.17(12)
O(12)-Mn(1)-N(41)	93.21(10)
O(11)-Mn(1)-N(41)	88.59(10)
N(11)-Mn(1)-N(41)	93.76(11)
N(12)-Mn(1)-N(41)	95.11(12)
O(12)-Mn(1)-O(401)	87.92(11)
O(11)-Mn(1)-O(401)	88.53(10)
N(11)-Mn(1)-O(401)	85.36(11)
N(12)-Mn(1)-O(401)	87.61(12)
N(41)-Mn(1)-O(401)	177.03(11)
Mn(2)-Mn(1)-Mn(1)#1	48.794(4)
C(1)-O(11)-Mn(1)	125.0(2)
C(101)-O(12)-Mn(1)	130.8(2)
C(41)-Mn(2)-C(41)#1	92.68(12)
C(41)-N(41)-Mn(1)	156.3(3)
N(41)-C(41)-Mn(2)	176.2(3)

Symmetry transformations used to generate equivalent atoms: #1 -y+3/4,-z+5/4,x+1/2 #2 z-1/2,-x+3/4,-y+5/4 #3 -x+1/2,-y+1,-z+3/2 #4 -z+1,x+1/4,y+1/4 #5 y-1/4,z-1/4,-x+1