

SUPPORTING INFORMATION

A Series of $[\text{NaMn}^{\text{III}}_3\text{Mn}^{\text{II}}]$ Clusters Constructed by Multidentate Schiff-Base Ligand and Decorated by Different Auxiliary Ligands

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Table S1. Bond Valence Sum Calculations for Compounds 1, 2, 3 and 4

Compounds	Mn	BVS
[NaMn ^{III} ₃ Mn ^{II} (HL) ₃ (μ ₄ -O)(μ _{1,1} -N ₃) ₃] ClO ₄ ·CH ₃ CH ₂ OH·(H ₂ O) ₃ (1)	Mn1	3.31535
	Mn2	3.30965
	Mn3	3.29588
	Mn4	2.07624
[NaMn ^{III} ₃ Mn ^{II} (HL) ₃ (μ ₄ -O)(μ _{1,1} -N ₃) ₂ (μ _{1,3} -N ₃)] ClO ₄ ·CH ₃ CH ₂ OH·H ₂ O (2)	Mn1	3.32426
	Mn2	3.33513
	Mn3	3.26671
	Mn4	2.05795
[NaMn ^{III} ₃ Mn ^{II} (HL) ₃ (μ ₄ -O)(HCOO) ₃] ClO ₄ ·4H ₂ O (3)	Mn1	3.4238
	Mn2	3.42369
	Mn3	3.4099
	Mn4	2.11774
[NaMn ^{III} ₃ Mn ^{II} (HL) ₃ (μ ₄ -O)(PhCOO)(H ₂ O) ₂] (ClO ₄) ₂ ·H ₂ O·PhCOO·PhCOOH·CH ₃ OH (4)	Mn1	3.10961
	Mn2	3.4323
	Mn3	3.52907
	Mn4	2.07104

Table S2. Selected Distances and Bond Angles for Cluster 1

Cluster		1	
Distances [Å]			
Mn1-N1	1.987(7)	Mn3-O11	1.880(5)
Mn1-N4	2.414(7)	Mn3-O13	1.872(5)
Mn1-N7	2.391(6)	Mn4-O3	2.136(6)
Mn1-O2	1.885(6)	Mn4-O4	2.271(13)
Mn1-O3	1.872(6)	Mn4-O7	2.137(6)
Mn1-O13	1.884(5)	Mn4-O8	2.222(7)
Mn2-N2	1.980(7)	Mn4-O11	2.136(5)
Mn2-N7	2.351(6)	Mn4-O12	2.234(10)
Mn2-N10	2.374(6)	Na1-O1	2.538(6)
Mn2-O6	1.892(6)	Na1-O2	2.390(6)
Mn2-O7	1.901(6)	Na1-O5	2.451(6)
Mn2-O13	1.878(5)	Na1-O6	2.419(6)
Mn3-N3	1.973(6)	Na1-O9	2.466(6)
Mn3-N4	2.426(7)	Na1-O10	2.376(5)
Mn3-N10	2.384(7)	Na1-O13	2.645(6)
Mn3-O10	1.892(5)		
Angles [°]			
N1-Mn1-N4	110.7(3)	O3-Mn4-O4	75.1(4)
N1-Mn1-N7	95.3(2)	O3-Mn4-O7	91.3(2)

O2-Mn1-N1	90.2(3)	O3-Mn4-O8	133.9(3)
O2-Mn1-N4	88.8(2)	O3-Mn4-O12	137.0(4)
O2-Mn1-N7	92.6(2)	O7-Mn4-O4	116.7(4)
O3-Mn1-N1	84.1(3)	O7-Mn4-O8	74.5(3)
O3-Mn1-N4	90.2(2)	O7-Mn4-O12	129.2(4)
O3-Mn1-N7	91.1(2)	O8-Mn4-O4	73.3(4)
O3-Mn1-O13	95.4(2)	O8-Mn4-O12	78.4(4)
O13-Mn1-N4	77.1(2)	O11-Mn4-O3	92.8(2)
O13-Mn1-N7	76.9(2)	O11-Mn4-O4	149.1(4)
O13-Mn1-O2	90.7(2)	O11-Mn4-O7	91.4(2)
N2-Mn2-N7	97.5(3)	O11-Mn4-O8	130.2(3)
N2-Mn2-N10	106.0(3)	O11-Mn4-O12	74.8(3)
O6-Mn2-N2	91.0(3)	O12-Mn4-O4	94.6(5)
O6-Mn2-N7	87.0(2)	O1-Na1-O13	126.1(2)
O6-Mn2-N10	94.2(2)	O2-Na1-O1	63.7(2)
O7-Mn2-N2	82.0(3)	O2-Na1-O5	108.7(2)
O7-Mn2-N7	92.9(2)	O2-Na1-O6	102.7(2)
O7-Mn2-N10	88.7(2)	O2-Na1-O9	140.8(2)
O13-Mn2-N7	78.1(2)	O2-Na1-O13	64.11(18)
O13-Mn2-N10	78.3(2)	O5-Na1-O1	83.8(2)
O13-Mn2-O6	91.9(2)	O5-Na1-O9	93.2(2)
O13-Mn2-O7	95.0(2)	O5-Na1-O13	125.5(2)
N3-Mn3-N4	99.0(3)	O6-Na1-O1	140.9(2)
N3-Mn3-N10	105.7(3)	O6-Na1-O5	65.4(2)
O10-Mn3-N3	91.2(2)	O6-Na1-O9	116.0(2)
O10-Mn3-N4	93.7(2)	O6-Na1-O13	64.51(18)
O10-Mn3-N10	90.0(2)	O9-Na1-O1	87.8(2)
O11-Mn3-N3	82.9(2)	O9-Na1-O13	127.39(19)
O11-Mn3-N4	87.7(2)	O10-Na1-O1	116.2(2)
O11-Mn3-N10	91.2(2)	O10-Na1-O2	102.5(2)
O13-Mn3-N4	77.0(2)	O10-Na1-O5	148.2(2)
O13-Mn3-N10	78.2(2)	O10-Na1-O6	102.3(2)
O13-Mn3-O10	90.5(2)	O10-Na1-O9	64.95(19)
O13-Mn3-O11	95.5(2)	O10-Na1-O13	64.05(17)

Table S3. Selected Distances and Bond Angles for Cluster 2

Cluster		2	
Distances [Å]			
Mn1-N1	1.988(4)	Mn3-O11	1.900(3)

Mn1-N4	2.309(5)	Mn3-O13	1.882(3)
Mn1-N12	2.316(5)	Mn4-O3	2.138(3)
Mn1-O2	1.896(3)	Mn4-O4	2.271(4)
Mn1-O3	1.898(3)	Mn4-O7	2.130(4)
Mn1-O13	1.895(3)	Mn4-O8	2.263(12)
Mn2-N2	1.979(4)	Mn4-O11	2.167(4)
Mn2-N4	2.290(4)	Mn4-O12	2.202(5)
Mn2-N7	2.334(4)	Na1-O1	2.500(4)
Mn2-O6	1.903(4)	Na1-O2	2.396(4)
Mn2-O7	1.904(4)	Na1-O5	2.515(4)
Mn2-O13	1.926(3)	Na1-O6	2.356(4)
Mn3-N3	1.970(4)	Na1-O9	2.533(4)
Mn3-N7	2.303(5)	Na1-O10	2.399(4)
Mn3-N10	2.382(5)	Na1-O13	2.689(4)
Mn3-O10	1.889(4)		
Angles [°]			
N1-Mn1-N4	90.68(18)	O3-Mn4-O8	141.4(4)
N1-Mn1-N12	89.54(18)	O3-Mn4-O11	98.49(13)
O2-Mn1-N1	91.07(17)	O3-Mn4-O12	135.92(19)
O2-Mn1-N4	92.16(16)	O7-Mn4-O3	91.16(14)
O2-Mn1-N12	88.87(16)	O7-Mn4-O4	132.38(15)
O3-Mn1-N1	84.04(17)	O7-Mn4-O8	74.9(3)
O3-Mn1-N4	89.32(16)	O7-Mn4-O11	87.34(14)
O3-Mn1-N12	89.67(16)	O7-Mn4-O12	130.36(18)
O13-Mn1-N4	83.35(15)	O7-Mn4-O8'	73.1(2)
O13-Mn1-N12	96.40(16)	O8-Mn4-O4	89.8(4)
O13-Mn1-O2	90.92(15)	O11-Mn4-O4	138.46(15)
O13-Mn1-O3	94.08(15)	O11-Mn4-O8	116.2(4)
N2-Mn2-N4	96.87(17)	O11-Mn4-O12	73.29(15)
N2-Mn2-N7	99.17(17)	O12-Mn4-O4	84.94(17)
O6-Mn2-N2	90.42(17)	O12-Mn4-O8	73.9(4)
O6-Mn2-N4	89.51(16)	O12-Mn4-O8'	88.3(3)
O6-Mn2-N7	93.43(15)	O8'-Mn4-O4	78.2(3)
O6-Mn2-O13	92.47(14)	O8'-Mn4-O8	19.3(3)
O7-Mn2-N2	83.27(17)	O1-Na1-O5	85.20(14)
O7-Mn2-N4	90.43(16)	O1-Na1-O9	91.21(13)
O7-Mn2-N7	88.41(15)	O1-Na1-O13	122.77(14)
O7-Mn2-O13	93.85(15)	O2-Na1-O1	64.51(13)
O13-Mn2-N4	83.21(15)	O2-Na1-O5	101.34(14)
O13-Mn2-N7	80.62(15)	O2-Na1-O9	151.30(14)

N3-Mn3-N7	99.03(18)	O2-Na1-O10	114.01(15)
N3-Mn3-N10	83.78(18)	O2-Na1-O13	63.88(12)
O10-Mn3-N3	92.27(17)	O5-Na1-O9	90.98(14)
O10-Mn3-N7	87.09(16)	O5-Na1-O13	127.71(13)
O10-Mn3-N10	87.60(16)	O6-Na1-O1	139.10(14)
O11-Mn3-N3	83.57(17)	O6-Na1-O2	93.19(14)
O11-Mn3-N7	94.63(16)	O6-Na1-O5	65.13(13)
O11-Mn3-N10	90.85(16)	O6-Na1-O9	115.50(15)
O13-Mn3-Na1	50.01(11)	O6-Na1-O10	99.35(14)
O13-Mn3-N7	82.33(15)	O6-Na1-O13	66.08(12)
O13-Mn3-N10	95.16(16)	O9-Na1-O13	126.82(13)
O13-Mn3-O10	91.01(15)	O10-Na1-O1	120.68(14)
O13-Mn3-O11	93.12(15)	O10-Na1-O9	63.99(13)
O3-Mn4-O4	73.10(14)	O10-Na1-O13	63.52(12)

Table S4. Selected Distances and Bond Angles for Cluster 3

Cluster		3	
Distances [Å]			
Mn1-N1	1.974(3)	Mn3-O17	2.217(2)
Mn1-O2	1.898(2)	Mn3-O20	1.882(2)
Mn1-O3	1.897(2)	Mn4-O3	2.141(2)
Mn1-O13	2.296(3)	Mn4-O4	2.241(6)
Mn1-O18	2.236(2)	Mn4-O7	2.148(2)
Mn1-O20	1.888(2)	Mn4-O8	2.202(6)
Mn2-N2	1.978(3)	Mn4-O11	2.131(2)
Mn2-O6	1.904(2)	Mn4-O12	2.234(10)
Mn2-O7	1.890(2)	Na-O1	2.508(2)
Mn2-O13	2.258(2)	Na-O2	2.403(3)
Mn2-O15	2.209(2)	Na-O6	2.373(3)
Mn2-O20	1.919(2)	Na-O9	2.553(3)
Mn3-N3	1.979(3)	Na-O10	2.387(3)
Mn3-O10	1.892(2)	Na-O19	2.499(3)
Mn3-O11	1.894(2)	Na-O20	2.690(2)
Mn3-O15	2.365(3)		
Angles [°]			
N1-Mn1-O13	95.48(11)	O3-Mn4-O4	72.51(15)
N1-Mn1-O18	89.63(11)	O3-Mn4-O7	89.59(9)
O2-Mn1-N1	91.58(10)	O3-Mn4-O8	112.5(2)
O2-Mn1-O13	88.67(9)	O3-Mn4-O12	136.5(2)
O2-Mn1-O18	89.66(9)	O7-Mn4-O4	144.92(19)
O3-Mn1-N1	83.44(10)	O7-Mn4-O8	74.82(16)
O3-Mn1-O13	92.21(9)	O7-Mn4-O12	132.2(2)

O3-Mn1-O18	89.89(9)	O8-Mn4-O4	84.4(2)
O20-Mn1-O2	91.89(9)	O8-Mn4-O12	93.0(3)
O20-Mn1-O3	93.11(9)	O11-Mn4-O3	98.19(9)
O20-Mn1-O13	79.19(9)	O11-Mn4-O4	121.8(2)
O20-Mn1-O18	95.80(9)	O11-Mn4-O7	89.85(9)
N2-Mn2-O13	93.81(11)	O11-Mn4-O8	145.2(2)
N2-Mn2-O15	105.32(11)	O11-Mn4-O12	74.3(3)
O6-Mn2-N2	91.06(11)	O12-Mn4-O4	75.8(3)
O6-Mn2-O13	92.03(9)	O1-Na-O9	90.86(8)
O6-Mn2-O15	89.29(9)	O1-Na-O20	128.24(8)
O6-Mn2-O20	91.29(9)	O2-Na-O1	64.26(8)
O7-Mn2-N2	82.99(11)	O2-Na-O9	127.33(10)
O7-Mn2-O13	89.29(10)	O2-Na-O19	133.60(9)
O7-Mn2-O15	91.40(10)	O2-Na-O20	64.30(7)
O7-Mn2-O20	94.73(10)	O6-Na-O1	117.68(9)
O20-Mn2-O13	79.56(9)	O6-Na-O2	98.13(9)
O20-Mn2-O15	81.27(9)	O6-Na-O9	134.13(10)
N3-Mn3-O15	91.85(10)	O6-Na-O10	98.02(9)
N3-Mn3-O17	90.10(10)	O6-Na-O19	64.11(8)
O10-Mn3-N3	91.35(10)	O6-Na-O20	65.01(8)
O10-Mn3-O15	92.37(10)	O9-Na-O20	125.44(8)
O10-Mn3-O17	88.61(10)	O10-Na-O1	144.22(10)
O11-Mn3-N3	83.80(10)	O10-Na-O2	110.71(9)
O11-Mn3-O15	88.68(10)	O10-Na-O9	63.31(8)
O11-Mn3-O17	90.51(10)	O10-Na-O19	113.94(9)
O20-Mn3-O10	90.64(9)	O10-Na-O20	63.49(8)
O20-Mn3-O11	94.29(9)	O19-Na-O1	85.78(8)
O20-Mn3-O15	77.94(9)	O19-Na-O9	84.87(9)
O20-Mn3-O17	100.09(9)	O19-Na-O20	127.93(9)

Table S5. Selected Distances and Bond Angles for Cluster 4

Cluster		4	
Distances [Å]			
Mn1-N1	1.953(8)	Mn3-O16	2.522(6)
Mn1-O2	1.885(6)	Mn3-O13	1.883(5)
Mn1-O3	1.877(6)	Mn4-O11	2.107(6)
Mn1-O14	2.125(5)	Mn4-O12	2.265(7)
Mn1-O17	2.523(6)	Mn4-O3	2.180(6)
Mn1-O13	1.884(6)	Mn4-O4	2.182(7)
Mn2-N2	1.976(7)	Mn4-O7	2.157(6)
Mn2-O6	1.885(5)	Mn4-O8	2.216(6)
Mn2-O7	1.874(5)	Na1-O9	2.448(8)
Mn2-O17	2.285(6)	Na1-O10	2.402(7)

Mn2-O16	2.328(6)	Na1-O1	2.532(7)
Mn2-O13	1.899(5)	Na1-O2	2.377(8)
Mn3-N3	1.970(7)	Na1-O5	2.539(8)
Mn3-O10	1.882(6)	Na1-O6	2.361(7)
Mn3-O11	1.892(5)	Na1-O13	2.658(6)
Mn3-O15	2.097(6)		

Angles [°]

N1-Mn1-O14	88.9(3)	O11-Mn4-O12	73.1(3)
N1-Mn1-O17	93.5(3)	O11-Mn4-O3	95.3(2)
O2-Mn1-N1	92.1(3)	O11-Mn4-O4	124.7(3)
O2-Mn1-O14	91.8(2)	O11-Mn4-O7	89.2(2)
O2-Mn1-O17	82.1(2)	O11-Mn4-O8	139.3(3)
O3-Mn1-N1	82.5(3)	O3-Mn4-O12	142.3(3)
O3-Mn1-O14	94.2(2)	O3-Mn4-O4	73.6(2)
O3-Mn1-O17	92.0(2)	O3-Mn4-O8	121.2(3)
O3-Mn1-O13	92.3(2)	O4-Mn4-O12	83.8(3)
O13-Mn1-O2	91.9(3)	O4-Mn4-O8	85.6(3)
O13-Mn1-O14	101.8(2)	O7-Mn4-O12	124.1(3)
O13-Mn1-O17	76.3(2)	O7-Mn4-O3	90.6(2)
N2-Mn2-O17	95.1(3)	O7-Mn4-O4	143.0(3)
N2-Mn2-O16	99.9(3)	O7-Mn4-O8	74.2(2)
O6-Mn2-N2	90.8(3)	O8-Mn4-O12	85.7(3)
O6-Mn2-O17	96.0(2)	O9-Na1-O1	98.9(3)
O6-Mn2-O16	88.2(2)	O9-Na1-O5	86.3(3)
O6-Mn2-O13	91.9(2)	O9-Na1-O13	123.4(2)
O7-Mn2-N2	82.9(3)	O10-Na1-O9	64.5(2)
O7-Mn2-O17	86.2(2)	O10-Na1-O5	105.4(3)
O7-Mn2-O16	91.4(2)	O10-Na1-O13	62.43(19)
O7-Mn2-O13	94.3(2)	O1-Na1-O5	87.3(3)
O13-Mn2-O17	82.3(2)	O1-Na1-O13	124.6(3)
O13-Mn2-O16	82.5(2)	O2-Na1-O9	119.9(3)
N3-Mn3-O15	87.6(3)	O2-Na1-O10	110.4(2)
N3-Mn3-O16	94.4(3)	O2-Na1-O1	63.4(2)
O10-Mn3-N3	91.5(3)	O2-Na1-O5	142.1(3)
O10-Mn3-O15	94.4(3)	O2-Na1-O13	64.8(2)
O10-Mn3-O16	91.7(2)	O5-Na1-O13	125.5(2)
O10-Mn3-O13	88.7(2)	O6-Na1-O9	141.2(3)
O11-Mn3-N3	83.5(3)	O6-Na1-O10	97.8(2)
O11-Mn3-O15	91.1(3)	O6-Na1-O1	104.2(2)
O11-Mn3-O16	83.0(2)	O6-Na1-O2	98.3(3)
O13-Mn3-O11	95.4(2)	O6-Na1-O5	64.4(2)
O13-Mn3-O15	100.3(2)	O6-Na1-O13	65.35(19)
O13-Mn3-O16	77.7(2)		
