Supporting Information

Synthesis, characterization and crystal structures of two new manganese aceto EMIM ionic compounds with chains of Mn^{2+} ions coordinated exclusively by acetate

Przemyslaw Dera[1]*, Edward Bruffey III[2], Gregory J. Finkelstein[1], Colleen Kelly[2], Angelina Gigante[3], Hans Hagemann[3], and Godwin Severa[2]*

[1]Hawai'i Institute of Geophysics and Planetology, University of Hawai'i at Mānoa, 1680 East West Rd, POST 109, Honolulu, HI, 96822, USA
[2]Hawai'i Natural Energy Institute, University of Hawai'i at Mānoa, 1680 East West Rd, POST 109, Honolulu, HI, 96822, USA
[3]Département de Chimie Physique, Université de Genève, 30, quai E. Ansermet, 1211 Geneva 4, Switzerland

Table S1. Hydrogen bond geometry parameters for compound **I**.

	H…A distance [Å]	**D…A distance [Å]**	**D-H distance [Å]**	**D-H…A angle [deg]**
Aromatic				
C4-H4 … O7	2.446(3)	3.309(7)	0.930(6)	154.5(4)
C2-H2 … O4	2.632(4)	3.119(7)	0.930(5)	113.3(4)
C2-H2 … O5	2.377(4)	3.229(7)	0.930(5)	152.2(3)
C3-H3 … O1	2.606(4)	3.076(6)	0.929(5)	111.9(3)
C3-H3 … O3	2.210(4)	3.122(7)	0.929(5)	167.0(3)
C3-H3 … O7	2.843(4)	3.077(6)	0.929(5)	95.6(3)
Ethyl chain				
C6-H6A	no hbonds			
C6-H6B	no hbonds			
C6-H6C	no hbonds			
C5-H5AB	no hbonds			
C5-H5A … O5	2.656(3)	3.545(7)	0.971(6)	152.4(4)
Methyl chain				
C1-H1A … O2	2.650(4)	3.574(7)	0.960(5)	161.7(3)
C1-H1B … O1	2.799(4)	3.503(6)	0.960(5)	130.9(3)
C1-H1B … O10_#1	2.606(4)	3.488(6)	0.960(5)	152.9(3)
C1-H1C … O6	2.694(5)	3.503(7)	0.960(5)	142.4(3)
C1-H1C … O8	2.831(4)	3.640(6)	0.960(5)	142.5(3)

Atom symmetry transformation codes from original coordinates:
#1: 0.5-x, -0.5+y, 0.5-z

Table S2. Hydrogen bond geometry parameters for compound **II**.

	H…A distance [Å]	**D…A distance [Å]**	**D-H distance [Å]**	**D-H…A angle [deg]**
EMIM aromatic hydrogens				
C10-H10 … O2	2.725(7)	3.495(10)	0.930(3)	140.70(2)
C10-H10 … O7	2.671(7)	3.088(8)	0.930(3)	108.04(2)
C10-H10 … O9	2.577(9)	3.396(14)	0.930(3)	147.08(2)
C10-H10 … O10	2.764(8)	3.165(11)	0.930(3)	107.05(1)
C11-H11 … O4	2.606(8)	3.197(7)	0.930(2)	121.95(2)
C11-H11 … O3	2.880(6)	3.610(8)	0.930(2)	136.27(2)
C12-H12 … O1	2.435(8)	3.344(11)	0.929(3)	165.82(2)
EMIM ethyl chain hydrogens				
C16-H16A no hbonds				
C16-H16B no hbonds				
C16-H16C no hbonds				
C15-H5AB no hbonds				
C15-H15A … O2	2.619(12)	3.475(15)	0.970(3)	147.26(2)
EMIM methyl chain hydrogens				
C9-H9A … O9	2.850(5)	3.511(10)	0.960(4)	126.85(2)
C9-H9B … O4	2.589(8)	3.432(8)	0.960(1)	146.59(2)
C9-H9B … O11	2.852(9)	3.678(10)	0.960(1)	144.66(2)
C9-H9C … O5	2.685(7)	3.471(9)	0.960(2)	139.53(2)

Table S3. Crystal data and structure refinement for compund I.

Identification code	Compund I
Empirical formula	C16 H26 Mn2 N2 O10
Formula weight	516.27
Temperature	373(2) K
Wavelength	0.56086 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 12.2690(8) A alpha = 90 deg. b = 9.2890(7) A beta = 92.724(2) deg. c = 21.0005(16) A gamma = 90 deg.
Volume	2390.7(3) A^3
Z, Calculated density	4, 1.434 Mg/m^3
Absorption coefficient	0.576 mm^-1
F(000)	1064
Crystal size	? x ? x ? mm
Theta range for data collection	2.281 to 20.018 deg.
Limiting indices	-14<=h<=14, -9<=k<=10, -25<=l<=25
Reflections collected / unique	19549 / 3645 [R(int) = 0.0595]
Completeness to theta = 19.665	83.5 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3645 / 251 / 292
Goodness-of-fit on F^2	1.116
Final R indices [I>2sigma(I)]	R1 = 0.0532, wR2 = 0.1036
R indices (all data)	R1 = 0.0707, wR2 = 0.1095
Largest diff. peak and hole	0.647 and -0.458 e.A^-3

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compund I.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn(1)	5000	5000	5000	19(1)
Mn(2)	2355(1)	3453(1)	4318(1)	23(1)
Mn(3)	0	5000	5000	24(1)
O(1)	4869(3)	2831(4)	5325(2)	28(1)
O(2)	3227(3)	2036(4)	4986(2)	30(1)
O(3)	4085(3)	4371(4)	4110(1)	23(1)
O(4)	3372(3)	2608(4)	3532(2)	30(1)
O(5)	1129(3)	1889(4)	4133(2)	31(1)
O(6)	-266(3)	2866(5)	4608(2)	47(1)
O(7)	1654(3)	4916(4)	3610(2)	30(1)
O(8)	276(3)	5920(4)	4099(2)	39(1)
O(9)	1790(3)	4654(4)	5111(2)	28(1)
O(10)	3434(3)	5469(4)	5398(2)	31(1)
N(1)	3433(3)	7721(5)	3007(2)	28(1)
N(2)	2763(3)	8423(5)	3881(2)	25(1)
C(1)	2445(4)	8453(6)	4544(2)	35(1)
C(2)	2515(4)	9451(6)	3432(2)	34(1)
C(3)	3318(4)	7394(6)	3617(2)	27(1)
C(4)	2931(4)	9011(6)	2883(3)	35(1)
C(5)	4061(5)	6897(7)	2556(3)	45(2)
C(6)	5255(5)	7288(9)	2615(4)	79(3)
C(7)	522(5)	6611(6)	3052(2)	38(1)
C(8)	849(4)	5745(6)	3633(2)	24(1)
C(9)	-502(5)	570(7)	4140(3)	47(2)
C(10)	172(4)	1875(6)	4310(2)	30(1)
C(11)	5243(5)	3094(9)	3421(3)	62(2)
C(12)	4166(4)	3357(6)	3697(2)	27(1)
C(13)	4265(5)	612(6)	5725(3)	38(1)
C(14)	4101(4)	1943(6)	5312(2)	25(1)
C(15)	2490(4)	5139(7)	5524(2)	32(1)
C(16A)	2080(30)	5720(90)	6167(18)	83(12)
C(16B)	2180(20)	5050(40)	6205(12)	36(6)

Table S5. Bond lengths [A] and angles [deg] for compund I.

Mn(1)-O(1)#1	2.136(3)
Mn(1)-O(1)	2.136(3)
Mn(1)-O(10)	2.176(3)
Mn(1)-O(10)#1	2.176(3)
Mn(1)-O(3)	2.213(3)
Mn(1)-O(3)#1	2.213(3)
Mn(2)-O(5)	2.114(4)
Mn(2)-O(9)	2.147(3)
Mn(2)-O(7)	2.162(3)
Mn(2)-O(2)	2.168(3)
Mn(2)-O(4)	2.257(3)
Mn(2)-O(3)	2.347(3)
Mn(2)-C(12)	2.630(5)
Mn(3)-O(8)#2	2.118(3)
Mn(3)-O(8)	2.118(3)
Mn(3)-O(6)	2.165(4)
Mn(3)-O(6)#2	2.165(4)
Mn(3)-O(9)	2.221(3)
Mn(3)-O(9)#2	2.221(3)
O(1)-C(14)	1.251(6)
O(2)-C(14)	1.248(6)
O(3)-C(12)	1.287(6)
O(4)-C(12)	1.234(6)
O(5)-C(10)	1.249(6)
O(6)-C(10)	1.248(6)
O(7)-C(8)	1.255(6)
O(8)-C(8)	1.242(6)
O(9)-C(15)	1.273(6)
O(10)-C(15)	1.238(6)
N(1)-C(3)	1.331(6)
N(1)-C(4)	1.367(7)
N(1)-C(5)	1.465(7)
N(2)-C(3)	1.311(6)
N(2)-C(2)	1.366(6)
N(2)-C(1)	1.464(6)
C(2)-C(4)	1.345(7)
C(5)-C(6)	1.509(9)
C(7)-C(8)	1.500(7)
C(9)-C(10)	1.501(7)
C(11)-C(12)	1.488(7)
C(13)-C(14)	1.518(7)
C(15)-C(16B)	1.50(3)
C(15)-C(16A)	1.56(3)
O(1)#1-Mn(1)-O(1)	180.0
O(1)#1-Mn(1)-O(10)	90.86(14)
O(1)-Mn(1)-O(10)	89.14(14)
O(1)#1-Mn(1)-O(10)#1	89.14(14)
O(1)-Mn(1)-O(10)#1	90.86(14)
O(10)-Mn(1)-O(10)#1	180.00(19)
O(1)#1-Mn(1)-O(3)	91.27(12)

O(1)-Mn(1)-O(3)	88.73(12)
O(10)-Mn(1)-O(3)	87.44(12)
O(10)#1-Mn(1)-O(3)	92.55(12)
O(1)#1-Mn(1)-O(3)#1	88.73(12)
O(1)-Mn(1)-O(3)#1	91.27(12)
O(10)-Mn(1)-O(3)#1	92.56(12)
O(10)#1-Mn(1)-O(3)#1	87.45(12)
O(3)-Mn(1)-O(3)#1	180.00(19)
O(5)-Mn(2)-O(9)	104.27(13)
O(5)-Mn(2)-O(7)	92.82(14)
O(9)-Mn(2)-O(7)	94.24(13)
O(5)-Mn(2)-O(2)	91.51(13)
O(9)-Mn(2)-O(2)	88.93(13)
O(7)-Mn(2)-O(2)	173.83(13)
O(5)-Mn(2)-O(4)	92.28(13)
O(9)-Mn(2)-O(4)	163.40(13)
O(7)-Mn(2)-O(4)	86.06(13)
O(2)-Mn(2)-O(4)	89.38(13)
O(5)-Mn(2)-O(3)	149.01(12)
O(9)-Mn(2)-O(3)	106.48(12)
O(7)-Mn(2)-O(3)	88.72(12)
O(2)-Mn(2)-O(3)	85.31(12)
O(4)-Mn(2)-O(3)	56.92(12)
O(5)-Mn(2)-C(12)	119.75(15)
O(9)-Mn(2)-C(12)	135.52(15)
O(7)-Mn(2)-C(12)	89.90(15)
O(2)-Mn(2)-C(12)	84.14(15)
O(4)-Mn(2)-C(12)	27.94(14)
O(3)-Mn(2)-C(12)	29.26(14)
O(8)#2-Mn(3)-O(8)	180.0
O(8)#2-Mn(3)-O(6)	86.70(16)
O(8)-Mn(3)-O(6)	93.30(16)
O(8)#2-Mn(3)-O(6)#2	93.30(16)
O(8)-Mn(3)-O(6)#2	86.70(16)
O(6)-Mn(3)-O(6)#2	180.0
O(8)#2-Mn(3)-O(9)	92.73(13)
O(8)-Mn(3)-O(9)	87.27(13)
O(6)-Mn(3)-O(9)	92.16(14)
O(6)#2-Mn(3)-O(9)	87.84(14)
O(8)#2-Mn(3)-O(9)#2	87.27(13)
O(8)-Mn(3)-O(9)#2	92.72(13)
O(6)-Mn(3)-O(9)#2	87.84(14)
O(6)#2-Mn(3)-O(9)#2	92.16(14)
O(9)-Mn(3)-O(9)#2	180.0
C(14)-O(1)-Mn(1)	133.1(3)
C(14)-O(2)-Mn(2)	141.4(3)
C(12)-O(3)-Mn(1)	135.3(3)
C(12)-O(3)-Mn(2)	87.7(3)
Mn(1)-O(3)-Mn(2)	111.44(13)
C(12)-O(4)-Mn(2)	93.1(3)
C(10)-O(5)-Mn(2)	128.6(3)
C(10)-O(6)-Mn(3)	143.6(3)
C(8)-O(7)-Mn(2)	130.4(3)
C(8)-O(8)-Mn(3)	140.5(4)

C(15)-O(9)-Mn(2)	118.7(3)
C(15)-O(9)-Mn(3)	130.7(3)
Mn(2)-O(9)-Mn(3)	110.37(14)
C(15)-O(10)-Mn(1)	152.1(4)
C(3)-N(1)-C(4)	108.3(4)
C(3)-N(1)-C(5)	125.9(5)
C(4)-N(1)-C(5)	125.6(5)
C(3)-N(2)-C(2)	108.7(4)
C(3)-N(2)-C(1)	125.7(4)
C(2)-N(2)-C(1)	125.6(4)
C(4)-C(2)-N(2)	107.3(5)
N(2)-C(3)-N(1)	108.8(4)
C(2)-C(4)-N(1)	106.9(5)
N(1)-C(5)-C(6)	111.0(5)
O(8)-C(8)-O(7)	125.8(5)
O(8)-C(8)-C(7)	115.6(5)
O(7)-C(8)-C(7)	118.6(4)
O(6)-C(10)-O(5)	125.1(5)
O(6)-C(10)-C(9)	118.0(5)
O(5)-C(10)-C(9)	116.9(5)
O(4)-C(12)-O(3)	121.2(4)
O(4)-C(12)-C(11)	120.1(5)
O(3)-C(12)-C(11)	118.7(5)
O(4)-C(12)-Mn(2)	59.0(2)
O(3)-C(12)-Mn(2)	63.1(2)
C(11)-C(12)-Mn(2)	170.1(5)
O(2)-C(14)-O(1)	126.4(5)
O(2)-C(14)-C(13)	117.1(5)
O(1)-C(14)-C(13)	116.5(4)
O(10)-C(15)-O(9)	123.4(4)
O(10)-C(15)-C(16B)	120.0(10)
O(9)-C(15)-C(16B)	115.9(10)
O(10)-C(15)-C(16A)	116.1(17)
O(9)-C(15)-C(16A)	118.6(14)

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

Table S6. Anisotropic displacement parameters (A^2 x 10^3) for compound I.

The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mn(1)	18(1)	22(1)	17(1)	-1(1)	0(1)	3(1)
Mn(2)	19(1)	30(1)	20(1)	0(1)	2(1)	5(1)
Mn(3)	15(1)	39(1)	18(1)	-2(1)	2(1)	5(1)
O(1)	27(2)	25(2)	32(2)	5(2)	-7(2)	-2(2)
O(2)	22(2)	32(2)	35(2)	9(2)	-5(2)	2(2)
O(3)	27(2)	23(2)	18(2)	-2(2)	-2(1)	2(2)
O(4)	22(2)	35(2)	34(2)	-13(2)	5(2)	-5(2)
O(5)	20(2)	36(2)	37(2)	-6(2)	4(2)	1(2)
O(6)	30(2)	49(3)	62(3)	-25(2)	16(2)	-5(2)
O(7)	31(2)	37(2)	22(2)	4(2)	1(2)	11(2)
O(8)	31(2)	61(3)	24(2)	11(2)	6(2)	13(2)
O(9)	17(2)	46(2)	22(2)	-5(2)	-1(1)	7(2)
O(10)	20(2)	43(2)	31(2)	-10(2)	6(2)	1(2)
N(1)	29(2)	28(3)	28(2)	-1(2)	-3(2)	-1(2)
N(2)	26(2)	23(2)	26(2)	5(2)	0(2)	0(2)
C(1)	43(3)	36(3)	26(3)	0(3)	3(2)	-2(3)
C(2)	41(3)	24(3)	36(3)	7(2)	3(3)	5(2)
C(3)	30(3)	21(3)	29(3)	-1(2)	-11(2)	-1(2)
C(4)	43(3)	35(3)	25(3)	7(2)	0(3)	-1(3)
C(5)	48(4)	50(4)	35(3)	-14(3)	-2(3)	6(3)
C(6)	47(4)	105(7)	86(6)	-52(5)	24(4)	4(4)
C(7)	40(3)	43(4)	31(3)	15(3)	4(2)	11(3)
C(8)	24(3)	28(3)	19(2)	1(2)	2(2)	-1(2)
C(9)	43(4)	54(4)	44(4)	-13(3)	17(3)	-18(3)
C(10)	29(3)	34(3)	26(3)	-3(2)	2(2)	-1(2)
C(11)	35(3)	112(6)	42(4)	-49(4)	13(3)	-16(4)
C(12)	24(3)	39(3)	19(2)	-5(2)	2(2)	0(2)
C(13)	44(4)	28(3)	41(3)	14(3)	-14(3)	-6(3)
C(14)	25(3)	25(3)	26(3)	-1(2)	3(2)	4(2)
C(15)	20(3)	52(4)	22(3)	-4(3)	-2(2)	9(3)
C(16A)	34(10)	190(40)	28(12)	-42(18)	0(8)	20(20)
C(16B)	12(7)	77(16)	18(5)	-6(9)	-4(5)	0(8)

Table S7. Crystal data and structure refinement for compund_ii.

Identification code	compund II
Empirical formula	C16 H28 Mn2 N2 O11
Formula weight	534.28
Temperature	573(2) K
Wavelength	0.56086 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.362(2) A alpha = 70.170(5) deg. b = 10.820(3) A beta = 87.581(5) deg. c = 12.659(3) A gamma = 79.631(6) deg.
Volume	1186.4(5) A^3
Z, Calculated density	2, 1.496 Mg/m^3
Absorption coefficient	0.583 mm^-1
F(000)	552
Crystal size	0.05 x 0.05 x 0.05 mm
Theta range for data collection	2.185 to 20.062 deg.
Limiting indices	-11<=h<=11, -13<=k<=12, -14<=l<=14
Reflections collected / unique	9848 / 3229 [R(int) = 0.0770]
Completeness to theta = 19.665	74.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3229 / 229 / 296
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0661, wR2 = 0.1493
R indices (all data)	R1 = 0.1143, wR2 = 0.1770
Largest diff. peak and hole	0.600 and -0.390 e.A^-3

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for compund II.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn(01)	5000	5000	0	35(1)
Mn(02)	5000	5000	5000	38(1)
Mn(03)	3605(1)	3837(1)	2931(1)	41(1)
O(1)	2007(7)	7851(7)	2717(6)	79(2)
O(2)	4779(7)	2905(6)	779(5)	57(2)
O(3)	3165(7)	2537(6)	2137(5)	63(2)
O(4)	2141(7)	3454(7)	4232(5)	64(2)
O(5)	2900(6)	4393(6)	5366(5)	57(2)
O(6)	6030(7)	2956(6)	5266(5)	56(2)
O(7)	5313(7)	2339(6)	3890(5)	58(2)
O(8)	4607(6)	5427(5)	3211(4)	44(1)
O(9)	5360(6)	5028(6)	1693(4)	47(1)
O(10)	7309(6)	4346(6)	-80(5)	52(2)
O(11)	7961(6)	4530(6)	-1841(5)	55(2)
N(1)	8971(7)	2635(7)	2785(6)	50(2)
N(2)	8425(9)	1040(8)	2337(7)	68(2)
C(1)	857(11)	3319(11)	5907(8)	70(3)
C(2)	2065(10)	3755(9)	5109(7)	48(2)
C(3)	6849(13)	739(9)	5329(9)	79(3)
C(4)	5989(9)	2131(8)	4784(7)	45(2)
C(5)	5870(12)	7011(10)	1936(8)	74(3)
C(6)	5266(8)	5734(8)	2290(7)	40(2)
C(7)	3552(13)	1095(10)	1089(9)	81(3)
C(8)	3851(10)	2268(8)	1363(7)	48(2)
C(9)	8853(11)	3909(11)	2927(10)	83(3)
C(10)	7966(10)	2246(9)	2366(7)	54(2)
C(11)	10153(10)	1635(10)	3066(9)	73(3)
C(12)	9814(11)	617(11)	2806(10)	80(3)
C(13)	8196(9)	4150(8)	-799(7)	44(2)
C(14)	9697(10)	3398(12)	-378(9)	88(4)
C(15)	7562(16)	248(13)	2000(15)	128(5)
C(16)	8180(30)	40(30)	980(20)	283(14)

Table S9. Bond lengths [A] and angles [deg] for compund_ii.

Mn(01)-O(10)#1	2.160(5)
Mn(01)-O(10)	2.160(5)
Mn(01)-O(2)	2.188(6)
Mn(01)-O(2)#1	2.188(6)
Mn(01)-O(9)	2.195(5)
Mn(01)-O(9)#1	2.195(5)
Mn(02)-O(6)	2.165(6)
Mn(02)-O(6)#2	2.165(6)
Mn(02)-O(5)#2	2.166(6)
Mn(02)-O(5)	2.166(6)
Mn(02)-O(8)	2.185(5)
Mn(02)-O(8)#2	2.186(5)
Mn(03)-O(4)	2.077(6)
Mn(03)-O(3)	2.088(6)
Mn(03)-O(7)	2.134(6)
Mn(03)-O(11)#1	2.182(6)
Mn(03)-O(8)	2.234(5)
Mn(03)-O(9)	2.448(6)
O(1)-H(1O1)	0.839(10)
O(1)-H(2O1)	0.838(11)
O(2)-C(8)	1.262(10)
O(3)-C(8)	1.237(10)
O(4)-C(2)	1.254(10)
O(5)-C(2)	1.250(10)
O(6)-C(4)	1.247(10)
O(7)-C(4)	1.252(10)
O(8)-C(6)	1.266(9)
O(9)-C(6)	1.234(9)
O(10)-C(13)	1.251(9)
O(11)-C(13)	1.257(9)
O(11)-Mn(03)#1	2.182(6)
N(1)-C(10)	1.296(11)
N(1)-C(11)	1.365(11)
N(1)-C(9)	1.434(12)
N(2)-C(10)	1.311(11)
N(2)-C(12)	1.385(12)
N(2)-C(15)	1.447(14)
C(1)-C(2)	1.515(12)
C(1)-H(1A)	0.9600
C(1)-H(1B)	0.9600
C(1)-H(1C)	0.9600
C(3)-C(4)	1.516(11)
C(3)-H(3A)	0.9600
C(3)-H(3B)	0.9600
C(3)-H(3C)	0.9600
C(5)-C(6)	1.506(12)
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(7)-C(8)	1.499(12)
C(7)-H(7A)	0.9600

C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(10)-H(10)	0.9300
C(11)-C(12)	1.343(14)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(14)	1.509(12)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-C(16)	1.46(2)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600

O(10)#1-Mn(01)-O(10)	180.0
O(10)#1-Mn(01)-O(2)	91.6(2)
O(10)-Mn(01)-O(2)	88.4(2)
O(10)#1-Mn(01)-O(2)#1	88.4(2)
O(10)-Mn(01)-O(2)#1	91.6(2)
O(2)-Mn(01)-O(2)#1	180.0
O(10)#1-Mn(01)-O(9)	91.7(2)
O(10)-Mn(01)-O(9)	88.3(2)
O(2)-Mn(01)-O(9)	87.7(2)
O(2)#1-Mn(01)-O(9)	92.3(2)
O(10)#1-Mn(01)-O(9)#1	88.3(2)
O(10)-Mn(01)-O(9)#1	91.7(2)
O(2)-Mn(01)-O(9)#1	92.3(2)
O(2)#1-Mn(01)-O(9)#1	87.7(2)
O(9)-Mn(01)-O(9)#1	180.0
O(6)-Mn(02)-O(6)#2	180.0(3)
O(6)-Mn(02)-O(5)#2	89.4(2)
O(6)#2-Mn(02)-O(5)#2	90.6(2)
O(6)-Mn(02)-O(5)	90.6(2)
O(6)#2-Mn(02)-O(5)	89.4(2)
O(5)#2-Mn(02)-O(5)	180.0
O(6)-Mn(02)-O(8)	93.1(2)
O(6)#2-Mn(02)-O(8)	86.9(2)
O(5)#2-Mn(02)-O(8)	90.1(2)
O(5)-Mn(02)-O(8)	89.9(2)
O(6)-Mn(02)-O(8)#2	86.9(2)
O(6)#2-Mn(02)-O(8)#2	93.1(2)
O(5)#2-Mn(02)-O(8)#2	89.9(2)
O(5)-Mn(02)-O(8)#2	90.1(2)
O(8)-Mn(02)-O(8)#2	180.0
O(4)-Mn(03)-O(3)	99.9(3)
O(4)-Mn(03)-O(7)	93.6(3)
O(3)-Mn(03)-O(7)	90.0(3)
O(4)-Mn(03)-O(11)#1	92.1(2)

O(3)-Mn(03)-O(11)#1	91.4(2)
O(7)-Mn(03)-O(11)#1	173.8(2)
O(4)-Mn(03)-O(8)	101.9(2)
O(3)-Mn(03)-O(8)	158.1(2)
O(7)-Mn(03)-O(8)	90.6(2)
O(11)#1-Mn(03)-O(8)	85.9(2)
O(4)-Mn(03)-O(9)	156.5(2)
O(3)-Mn(03)-O(9)	103.1(2)
O(7)-Mn(03)-O(9)	91.1(2)
O(11)#1-Mn(03)-O(9)	82.8(2)
O(8)-Mn(03)-O(9)	55.03(19)
H(1O1)-O(1)-H(2O1)	107(3)
C(8)-O(2)-Mn(01)	136.7(6)
C(8)-O(3)-Mn(03)	126.8(6)
C(2)-O(4)-Mn(03)	129.9(6)
C(2)-O(5)-Mn(02)	142.7(6)
C(4)-O(6)-Mn(02)	135.4(5)
C(4)-O(7)-Mn(03)	135.2(6)
C(6)-O(8)-Mn(02)	140.0(5)
C(6)-O(8)-Mn(03)	96.2(5)
Mn(02)-O(8)-Mn(03)	111.0(2)
C(6)-O(9)-Mn(01)	145.2(5)
C(6)-O(9)-Mn(03)	87.1(5)
Mn(01)-O(9)-Mn(03)	107.7(2)
C(13)-O(10)-Mn(01)	137.4(5)
C(13)-O(11)-Mn(03)#1	131.1(6)
C(10)-N(1)-C(11)	108.8(9)
C(10)-N(1)-C(9)	125.3(8)
C(11)-N(1)-C(9)	125.8(8)
C(10)-N(2)-C(12)	107.5(9)
C(10)-N(2)-C(15)	125.5(9)
C(12)-N(2)-C(15)	126.6(9)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(5)-C(2)-O(4)	125.0(8)
O(5)-C(2)-C(1)	117.9(9)
O(4)-C(2)-C(1)	117.1(8)
C(4)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
O(6)-C(4)-O(7)	126.5(8)
O(6)-C(4)-C(3)	116.9(8)
O(7)-C(4)-C(3)	116.6(8)
C(6)-C(5)-H(5A)	109.5
C(6)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(6)-C(5)-H(5C)	109.5

H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
O(9)-C(6)-O(8)	120.5(8)
O(9)-C(6)-C(5)	121.9(8)
O(8)-C(6)-C(5)	117.5(8)
C(8)-C(7)-H(7A)	109.5
C(8)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(8)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
O(3)-C(8)-O(2)	125.4(8)
O(3)-C(8)-C(7)	117.5(8)
O(2)-C(8)-C(7)	117.1(8)
N(1)-C(9)-H(9A)	109.5
N(1)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
N(1)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N(1)-C(10)-N(2)	110.1(8)
N(1)-C(10)-H(10)	124.9
N(2)-C(10)-H(10)	124.9
C(12)-C(11)-N(1)	106.9(9)
C(12)-C(11)-H(11)	126.6
N(1)-C(11)-H(11)	126.6
C(11)-C(12)-N(2)	106.7(9)
C(11)-C(12)-H(12)	126.7
N(2)-C(12)-H(12)	126.7
O(10)-C(13)-O(11)	126.2(8)
O(10)-C(13)-C(14)	117.0(8)
O(11)-C(13)-C(14)	116.8(8)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(2)-C(15)-C(16)	108.1(15)
N(2)-C(15)-H(15A)	110.1
C(16)-C(15)-H(15A)	110.1
N(2)-C(15)-H(15B)	110.1
C(16)-C(15)-H(15B)	110.1
H(15A)-C(15)-H(15B)	108.4
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

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

Table S10. Anisotropic displacement parameters (A^2 x 10^3) for compund II.

The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mn(01)	37(1)	39(1)	27(1)	-11(1)	-2(1)	-2(1)
Mn(02)	45(1)	43(1)	26(1)	-13(1)	-2(1)	-6(1)
Mn(03)	44(1)	47(1)	34(1)	-15(1)	-2(1)	-9(1)
O(1)	67(5)	74(5)	89(5)	-26(4)	-13(4)	10(4)
O(2)	58(4)	44(3)	62(4)	-8(3)	1(3)	-8(3)
O(3)	82(5)	73(4)	50(4)	-32(3)	5(3)	-33(4)
O(4)	63(4)	90(5)	49(4)	-30(3)	11(3)	-31(3)
O(5)	52(4)	74(4)	53(4)	-29(3)	8(3)	-17(3)
O(6)	67(4)	44(3)	53(4)	-18(3)	-12(3)	4(3)
O(7)	70(4)	52(3)	46(3)	-16(3)	-19(3)	9(3)
O(8)	56(4)	50(3)	26(3)	-11(2)	-2(2)	-12(3)
O(9)	44(3)	64(4)	36(3)	-22(3)	-3(2)	-5(3)
O(10)	36(3)	69(4)	44(3)	-17(3)	-2(3)	8(3)
O(11)	48(4)	74(4)	39(3)	-22(3)	-5(3)	5(3)
N(1)	36(4)	48(4)	55(4)	-6(4)	-6(3)	0(3)
N(2)	56(5)	49(5)	89(6)	-16(4)	-20(4)	4(4)
C(1)	68(7)	82(7)	54(6)	-15(5)	19(5)	-20(5)
C(2)	53(5)	51(5)	37(4)	-7(4)	-3(4)	-16(4)
C(3)	111(9)	43(5)	72(7)	-15(5)	-36(6)	17(5)
C(4)	44(5)	39(4)	44(5)	-10(4)	-2(4)	2(4)
C(5)	92(8)	82(7)	56(6)	-16(5)	7(6)	-49(6)
C(6)	29(4)	54(5)	34(4)	-15(4)	-8(3)	-3(4)
C(7)	127(10)	70(7)	65(7)	-36(6)	15(7)	-45(7)
C(8)	60(6)	45(5)	38(5)	-10(4)	-6(4)	-14(4)
C(9)	68(7)	79(7)	115(9)	-52(7)	-5(7)	-7(6)
C(10)	46(5)	53(5)	50(5)	-3(4)	-11(4)	0(4)
C(11)	34(5)	69(6)	101(8)	-16(6)	-19(5)	5(4)
C(12)	55(6)	53(6)	111(9)	-7(6)	-22(6)	8(5)
C(13)	44(5)	42(5)	44(5)	-13(4)	-7(4)	2(4)
C(14)	46(6)	132(10)	63(7)	-22(7)	-5(5)	23(6)
C(15)	110(10)	85(8)	194(14)	-59(10)	-80(10)	11(8)
C(16)	310(30)	370(30)	320(30)	-260(30)	10(20)	-150(30)