Supporting Information:

Consequences of Electron-Density Manipulations on the X-Ray Photoelectron Spectroscopic Properties of Ferrocenyl-β-diketonato Complexes of Manganese(III). Structure of [Mn(FcCOCHCOCH$_3$)$_3$]

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Content.

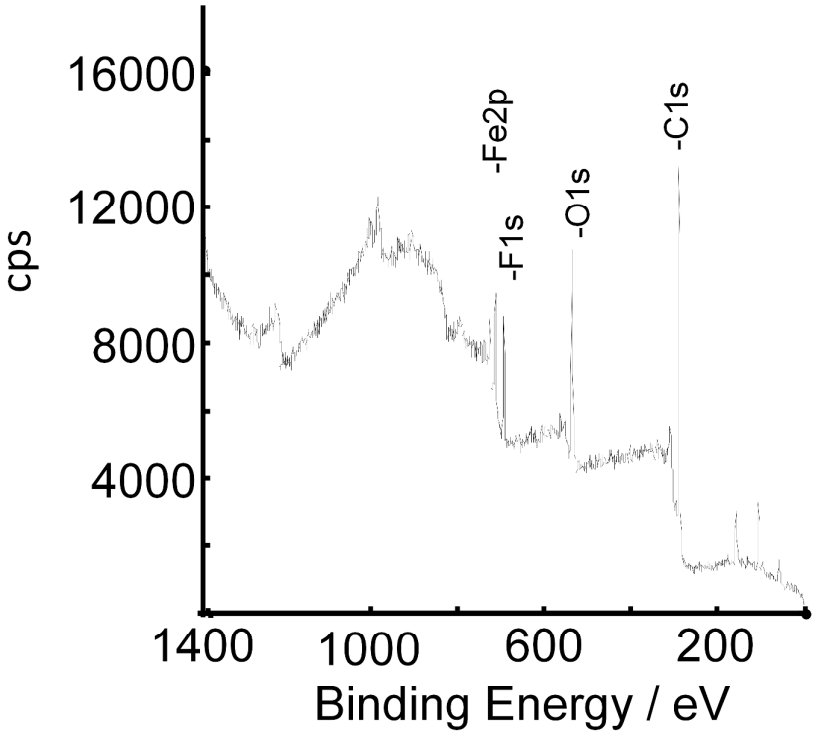

Fig. 1S Wide scan XPS spectrum of $FcCOCH_2COCF_3$

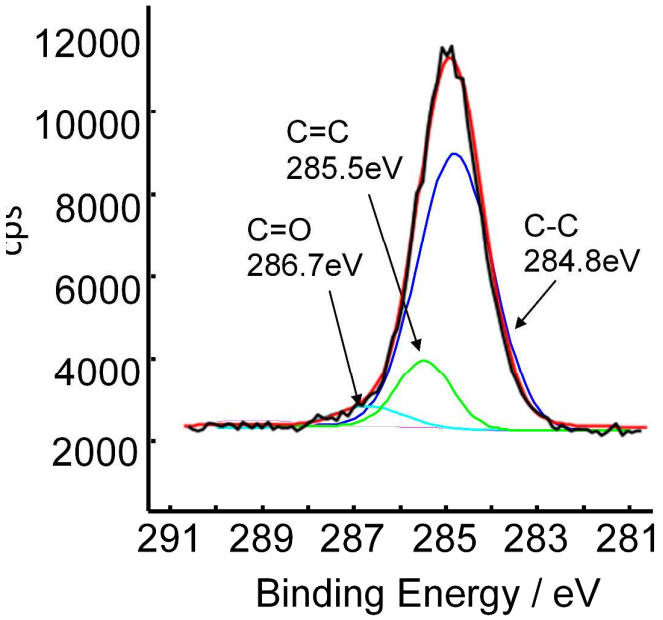

Fig. 2S Carbon 1S spectrum of of $FcCOCH_2COCF_3$

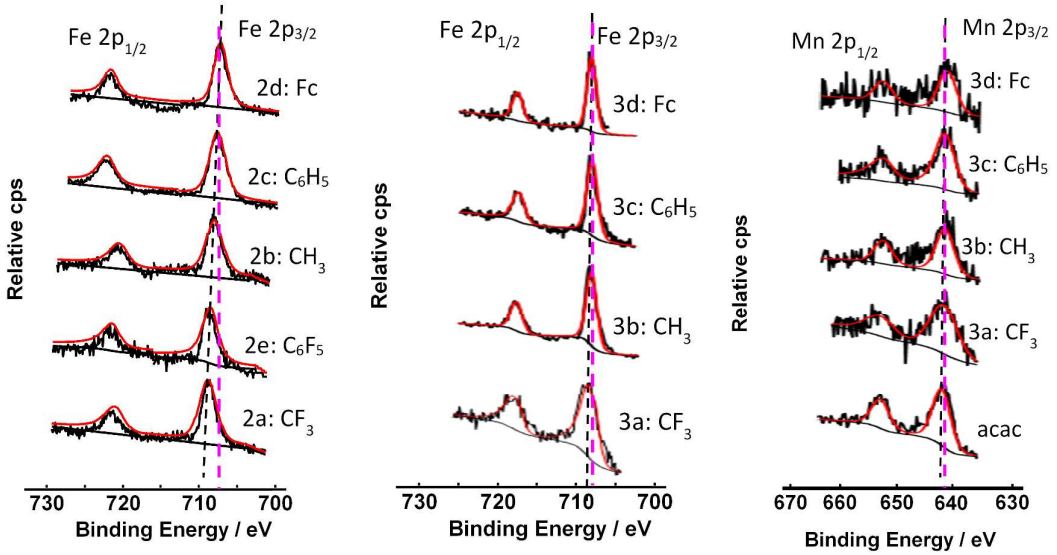

Fig. 3S Comparative XPS spectra showing the goodness-of-fits (red lines) to the experimentally obtained peak (black line of the Fe 2p area of (left) free β-diketones $FcCOCH_2COR$, **2a** – **2e**, and of (middle) the Fe 2p area of $Mn(FcCOCHCOR)_3$ complexes **3a** – **3d** and (right) of the Mn 2p area of **3a** – **3d**. The figure on the right also shows the XPS for $Mn(H_3CCOCHCOCH_3)_3$; it is labeled "acac". The dotted lines enhances BE changes: The move lines are absolutely vertical and the black lines follow the BE changes as good as possible.

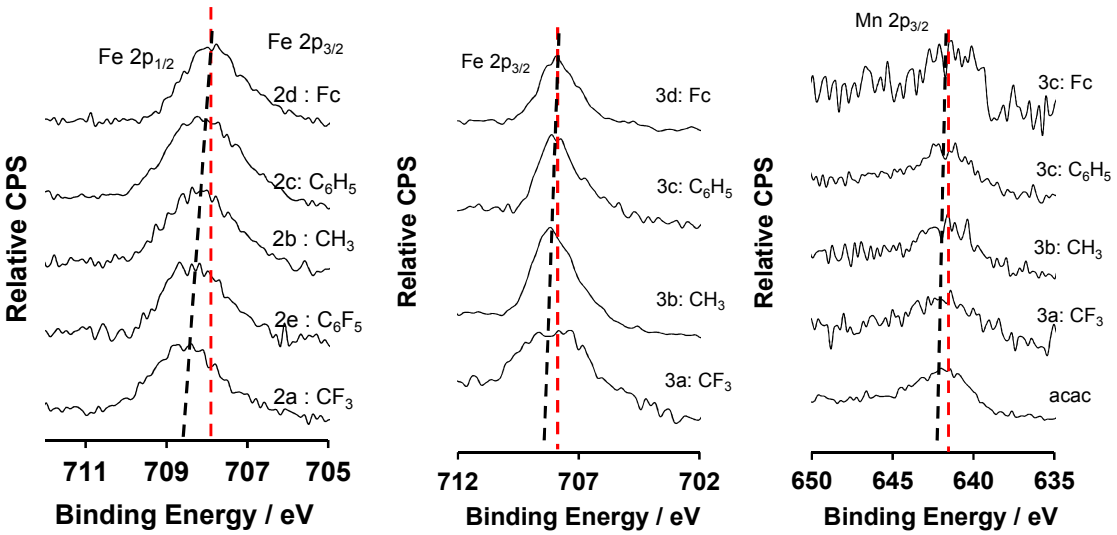

Fig. 4S Comparative XPS spectra of the Fe $2p_{3/2}$ area of (left) free β-diketones $FcCOCH_2COR$, **2a**–**2e**, and of (middle) the Fe $2p_{3/2}$ area of $[Mn(FcCOCHCOR)_3]$ complexes **3a**–**3d** and (right) of the Mn $2p_{3/2}$ area of **3a**–**3d**. The figure on the right also shows the XPS for $[Mn(H_3CCOCHCOCH_3)_3]$; it is labeled "acac". (CPS = counts per second.) The dotted lines enhance Binding Energy (BE) changes as a result of the influence of different R groups: Fc, C_6H_5, CH_3, CF_3. The red lines are absolutely vertical and the black lines follow the BE changes as good as possible.

5. Crystallographic data foe **3b.**

Table 1S. Crystal data and structure refinement for **3b**.

Empirical formula	$C_{45.29}H_{42.29}Fe_3MnO_6$	
Formula weight	905.11	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.7776(3) Å	α= 107.596(2)°.
	b = 14.1725(5) Å	β= 106.553(2)°.
	c = 14.9765(5) Å	γ = 107.047(2)°.
Volume	1901.60(11) $Å^3$	
Z	2	
Density (calculated)	1.581 Mg/m^3	
Absorption coefficient	1.497 mm^{-1}	
F(000)	930	
Crystal size	0.406 x 0.208 x 0.206 mm^3	
Theta range for data collection	2.512 to 25.679°.	
Index ranges	-13<=h<=13, -17<=k<=17, -18<=l<=18	
Reflections collected	66050	
Independent reflections	7212 [R(int) = 0.1009]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7212 / 0 / 484	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0534, wR2 = 0.1138	
R indices (all data)	R1 = 0.0795, wR2 = 0.1263	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.447 and -1.132 $e.Å^{-3}$	

Table 2S. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(1)	6400(1)	6616(1)	4078(1)	15(1)
Fe(1)	6713(1)	4024(1)	775(1)	22(1)
Fe(2)	2622(1)	8259(1)	3321(1)	21(1)
Fe(3)	11472(1)	9390(1)	7265(1)	25(1)
O(1)	7409(3)	6297(2)	3183(2)	22(1)
O(2)	7406(3)	6008(3)	4928(2)	24(1)
O(3)	5335(3)	7165(2)	3188(2)	21(1)
O(4)	4784(3)	5129(3)	3201(2)	25(1)
O(5)	7931(3)	8125(3)	5011(2)	22(1)
O(6)	5420(3)	6858(3)	5004(2)	23(1)
C(1)	8228(5)	4755(4)	5298(4)	30(1)
C(2)	7863(4)	5288(4)	4609(3)	22(1)
C(3)	8047(5)	5016(4)	3698(3)	22(1)
C(4)	7857(4)	5546(4)	3050(3)	21(1)
C(5)	2420(6)	3844(5)	2401(5)	39(1)
C(6)	3468(5)	4912(4)	2703(3)	23(1)
C(7)	3063(5)	5692(4)	2433(3)	21(1)
C(8)	3971(5)	6749(4)	2687(3)	19(1)
C(9)	5171(5)	7269(4)	6571(4)	30(1)
C(10)	6029(5)	7465(4)	5976(3)	21(1)
C(11)	7417(5)	8280(4)	6478(3)	21(1)
C(12)	8281(5)	8586(3)	5975(3)	18(1)
C(13)	8196(5)	5240(4)	2147(3)	23(1)
C(14)	8685(5)	4414(4)	1797(4)	30(1)
C(15)	8733(5)	4349(5)	854(4)	33(1)
C(16)	8255(5)	5098(4)	591(4)	34(1)
C(17)	7943(5)	5663(4)	1395(4)	26(1)
C(21)	5399(5)	2498(4)	-348(4)	36(1)
C(22)	4900(5)	3257(4)	-546(4)	34(1)
C(23)	4626(5)	3782(4)	295(4)	26(1)
C(24)	4975(5)	3354(4)	1022(4)	30(1)
C(25)	5442(5)	2551(4)	626(4)	36(1)
C(31)	3379(5)	7476(4)	2392(3)	20(1)

C(32)	4158(5)	8629(4)	2785(4)	24(1)
C(33)	3181(6)	9076(4)	2479(4)	33(1)
C(34)	1806(6)	8203(4)	1888(4)	33(1)
C(35)	1917(5)	7222(4)	1832(3)	26(1)
C(41)	2897(5)	7750(4)	4465(4)	24(1)
C(42)	3584(5)	8895(4)	4893(3)	25(1)
C(43)	2546(6)	9293(4)	4585(4)	32(1)
C(44)	1214(6)	8376(5)	3966(4)	35(1)
C(45)	1429(5)	7432(4)	3899(4)	30(1)
C(51)	9660(5)	9535(4)	6589(3)	20(1)
C(52)	10677(5)	9917(4)	6200(4)	26(1)
C(53)	11897(5)	10795(4)	7035(4)	33(1)
C(54)	11654(5)	10949(4)	7934(4)	33(1)
C(55)	10289(5)	10177(4)	7676(4)	25(1)
C(61)	11861(7)	8118(5)	6527(6)	55(1)
C(62)	13112(8)	8950(5)	7341(6)	55(1)
C(63)	12953(7)	9150(5)	8257(6)	55(1)
C(64)	11580(7)	8406(5)	8013(6)	55(1)
C(65)	10903(8)	7778(5)	6941(6)	55(1)
C(71)	1322(13)	-44(11)	300(6)	89(3)
C(72)	1241(14)	929(10)	369(6)	97(4)
C(73)	-54(12)	957(7)	79(6)	73(3)
C(74)	2720(20)	88(18)	563(12)	117(10)

Table 3S. Bond lengths [Å] and angles [°] for **3b**.

Mn(1)-O(6)	1.979(3)
Mn(1)-O(1)	1.984(3)
Mn(1)-O(2)	1.991(3)
Mn(1)-O(3)	1.994(3)
Mn(1)-O(5)	2.014(3)
Mn(1)-O(4)	2.018(3)
Fe(1)-C(24)	2.027(5)
Fe(1)-C(14)	2.027(5)
Fe(1)-C(13)	2.030(5)
Fe(1)-C(25)	2.037(5)
Fe(1)-C(21)	2.039(5)
Fe(1)-C(22)	2.041(5)
Fe(1)-C(16)	2.048(5)
Fe(1)-C(15)	2.049(5)
Fe(1)-C(23)	2.042(5)
Fe(1)-C(17)	2.051(5)
Fe(2)-C(31)	2.019(4)
Fe(2)-C(35)	2.028(5)
Fe(2)-C(41)	2.031(5)
Fe(2)-C(45)	2.034(5)
Fe(2)-C(44)	2.038(5)
Fe(2)-C(32)	2.041(5)
Fe(2)-C(34)	2.041(5)
Fe(2)-C(33)	2.050(5)
Fe(2)-C(42)	2.051(5)
Fe(2)-C(43)	2.054(5)
Fe(3)-C(62)	2.025(6)
Fe(3)-C(51)	2.027(4)
Fe(3)-C(55)	2.028(5)
Fe(3)-C(63)	2.036(6)
Fe(3)-C(61)	2.037(7)
Fe(3)-C(52)	2.037(5)
Fe(3)-C(65)	2.043(6)
Fe(3)-C(64)	2.045(6)
Fe(3)-C(54)	2.054(5)
Fe(3)-C(53)	2.064(5)

O(1)-C(4)	1.278(5)
O(2)-C(2)	1.283(5)
O(3)-C(8)	1.291(5)
O(4)-C(6)	1.291(5)
O(5)-C(12)	1.276(5)
O(6)-C(10)	1.287(5)
C(1)-C(2)	1.485(7)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.390(6)
C(3)-C(4)	1.401(6)
C(3)-H(3)	0.9500
C(4)-C(13)	1.473(6)
C(5)-C(6)	1.437(7)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-C(7)	1.424(7)
C(7)-C(8)	1.390(6)
C(7)-H(7)	0.9500
C(8)-C(31)	1.472(6)
C(9)-C(10)	1.480(7)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.400(6)
C(11)-C(12)	1.407(6)
C(11)-H(11)	0.9500
C(12)-C(51)	1.472(6)
C(13)-C(17)	1.425(7)
C(13)-C(14)	1.440(7)
C(14)-C(15)	1.404(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.416(8)
C(15)-H(15)	0.9500
C(16)-C(17)	1.418(7)
C(16)-H(16)	0.9500

C(17)-H(17)	0.9500
C(21)-C(22)	1.405(8)
C(21)-C(25)	1.423(8)
C(21)-H(21)	0.9500
C(22)-C(23)	1.415(7)
C(22)-H(22)	0.9500
C(23)-C(24)	1.412(7)
C(23)-H(23)	0.9500
C(24)-C(25)	1.414(7)
C(24)-H(24)	0.9500
C(25)-H(25)	0.9500
C(31)-C(35)	1.431(6)
C(31)-C(32)	1.433(7)
C(32)-C(33)	1.418(7)
C(32)-H(32)	0.9500
C(33)-C(34)	1.423(8)
C(33)-H(33)	0.9500
C(34)-C(35)	1.410(7)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500
C(41)-C(42)	1.409(7)
C(41)-C(45)	1.418(7)
C(41)-H(41)	0.9500
C(42)-C(43)	1.421(7)
C(42)-H(42)	0.9500
C(43)-C(44)	1.424(8)
C(43)-H(43)	0.9500
C(44)-C(45)	1.403(7)
C(44)-H(44)	0.9500
C(45)-H(45)	0.9500
C(51)-C(52)	1.428(6)
C(51)-C(55)	1.432(6)
C(52)-C(53)	1.415(7)
C(52)-H(52)	0.9500
C(53)-C(54)	1.410(8)
C(53)-H(53)	0.9500
C(54)-C(55)	1.410(7)
C(54)-H(54)	0.9500

C(55)-H(55)	0.9500
C(61)-C(65)	1.392(9)
C(61)-C(62)	1.398(10)
C(61)-H(61)	0.9500
C(62)-C(63)	1.385(10)
C(62)-H(62)	0.9500
C(63)-C(64)	1.407(9)
C(63)-H(63)	0.9500
C(64)-C(65)	1.410(10)
C(64)-H(64)	0.9500
C(65)-H(65)	0.9500
C(71)-C(72)	1.382(14)
C(71)-C(74)	1.39(2)
C(71)-C(73)#1	1.393(14)
C(72)-C(73)	1.355(14)
C(72)-H(72)	0.9500
C(73)-C(71)#1	1.393(14)
C(73)-H(73)	0.9500
C(74)-H(74A)	0.9800
C(74)-H(74C)	0.9800
C(74)-H(74B)	0.9800

O(6)-Mn(1)-O(1)	175.93(13)
O(6)-Mn(1)-O(2)	88.04(13)
O(1)-Mn(1)-O(2)	88.16(12)
O(6)-Mn(1)-O(3)	92.15(13)
O(1)-Mn(1)-O(3)	91.58(13)
O(2)-Mn(1)-O(3)	177.71(13)
O(6)-Mn(1)-O(5)	87.81(13)
O(1)-Mn(1)-O(5)	93.67(13)
O(2)-Mn(1)-O(5)	90.35(13)
O(3)-Mn(1)-O(5)	91.94(13)
O(6)-Mn(1)-O(4)	88.11(13)
O(1)-Mn(1)-O(4)	90.44(13)
O(2)-Mn(1)-O(4)	90.10(13)
O(3)-Mn(1)-O(4)	87.62(13)
O(5)-Mn(1)-O(4)	175.87(13)
C(24)-Fe(1)-C(14)	120.3(2)

C(24)-Fe(1)-C(13)	106.32(19)
C(14)-Fe(1)-C(13)	41.56(19)
C(24)-Fe(1)-C(25)	40.7(2)
C(14)-Fe(1)-C(25)	106.2(2)
C(13)-Fe(1)-C(25)	123.2(2)
C(24)-Fe(1)-C(21)	68.5(2)
C(14)-Fe(1)-C(21)	123.5(2)
C(13)-Fe(1)-C(21)	160.6(2)
C(25)-Fe(1)-C(21)	40.9(2)
C(24)-Fe(1)-C(22)	68.4(2)
C(14)-Fe(1)-C(22)	160.6(2)
C(13)-Fe(1)-C(22)	157.0(2)
C(25)-Fe(1)-C(22)	68.3(2)
C(21)-Fe(1)-C(22)	40.3(2)
C(24)-Fe(1)-C(16)	161.5(2)
C(14)-Fe(1)-C(16)	68.5(2)
C(13)-Fe(1)-C(16)	68.66(19)
C(25)-Fe(1)-C(16)	156.9(2)
C(21)-Fe(1)-C(16)	122.1(2)
C(22)-Fe(1)-C(16)	108.8(2)
C(24)-Fe(1)-C(15)	156.1(2)
C(14)-Fe(1)-C(15)	40.29(19)
C(13)-Fe(1)-C(15)	68.49(18)
C(25)-Fe(1)-C(15)	121.2(2)
C(21)-Fe(1)-C(15)	108.2(2)
C(22)-Fe(1)-C(15)	125.4(2)
C(16)-Fe(1)-C(15)	40.4(2)
C(24)-Fe(1)-C(23)	40.6(2)
C(14)-Fe(1)-C(23)	156.5(2)
C(13)-Fe(1)-C(23)	121.00(19)
C(25)-Fe(1)-C(23)	68.3(2)
C(21)-Fe(1)-C(23)	68.1(2)
C(22)-Fe(1)-C(23)	40.6(2)
C(16)-Fe(1)-C(23)	125.4(2)
C(15)-Fe(1)-C(23)	162.1(2)
C(24)-Fe(1)-C(17)	124.2(2)
C(14)-Fe(1)-C(17)	69.0(2)
C(13)-Fe(1)-C(17)	40.88(19)

C(25)-Fe(1)-C(17)	160.6(2)
C(21)-Fe(1)-C(17)	157.3(2)
C(22)-Fe(1)-C(17)	122.3(2)
C(16)-Fe(1)-C(17)	40.5(2)
C(15)-Fe(1)-C(17)	68.0(2)
C(23)-Fe(1)-C(17)	108.3(2)
C(31)-Fe(2)-C(35)	41.40(18)
C(31)-Fe(2)-C(41)	105.32(19)
C(35)-Fe(2)-C(41)	122.1(2)
C(31)-Fe(2)-C(45)	119.2(2)
C(35)-Fe(2)-C(45)	105.2(2)
C(41)-Fe(2)-C(45)	40.84(19)
C(31)-Fe(2)-C(44)	155.1(2)
C(35)-Fe(2)-C(44)	120.2(2)
C(41)-Fe(2)-C(44)	68.2(2)
C(45)-Fe(2)-C(44)	40.3(2)
C(31)-Fe(2)-C(32)	41.35(18)
C(35)-Fe(2)-C(32)	69.2(2)
C(41)-Fe(2)-C(32)	121.20(19)
C(45)-Fe(2)-C(32)	156.13(19)
C(44)-Fe(2)-C(32)	162.5(2)
C(31)-Fe(2)-C(34)	68.86(19)
C(35)-Fe(2)-C(34)	40.6(2)
C(41)-Fe(2)-C(34)	159.2(2)
C(45)-Fe(2)-C(34)	123.2(2)
C(44)-Fe(2)-C(34)	108.2(2)
C(32)-Fe(2)-C(34)	68.4(2)
C(31)-Fe(2)-C(33)	69.08(19)
C(35)-Fe(2)-C(33)	68.8(2)
C(41)-Fe(2)-C(33)	157.7(2)
C(45)-Fe(2)-C(33)	160.9(2)
C(44)-Fe(2)-C(33)	125.8(2)
C(32)-Fe(2)-C(33)	40.57(19)
C(34)-Fe(2)-C(33)	40.7(2)
C(31)-Fe(2)-C(42)	123.33(19)
C(35)-Fe(2)-C(42)	159.42(19)
C(41)-Fe(2)-C(42)	40.39(19)
C(45)-Fe(2)-C(42)	68.2(2)

C(44)-Fe(2)-C(42)	68.2(2)
C(32)-Fe(2)-C(42)	108.5(2)
C(34)-Fe(2)-C(42)	159.2(2)
C(33)-Fe(2)-C(42)	123.6(2)
C(31)-Fe(2)-C(43)	161.2(2)
C(35)-Fe(2)-C(43)	157.1(2)
C(41)-Fe(2)-C(43)	68.2(2)
C(45)-Fe(2)-C(43)	68.2(2)
C(44)-Fe(2)-C(43)	40.7(2)
C(32)-Fe(2)-C(43)	125.6(2)
C(34)-Fe(2)-C(43)	123.4(2)
C(33)-Fe(2)-C(43)	109.8(2)
C(42)-Fe(2)-C(43)	40.50(19)
C(62)-Fe(3)-C(51)	157.1(2)
C(62)-Fe(3)-C(55)	160.9(3)
C(51)-Fe(3)-C(55)	41.36(18)
C(62)-Fe(3)-C(63)	39.9(3)
C(51)-Fe(3)-C(63)	160.4(2)
C(55)-Fe(3)-C(63)	124.3(2)
C(62)-Fe(3)-C(61)	40.3(3)
C(51)-Fe(3)-C(61)	120.6(2)
C(55)-Fe(3)-C(61)	157.0(2)
C(63)-Fe(3)-C(61)	68.1(3)
C(62)-Fe(3)-C(52)	122.2(2)
C(51)-Fe(3)-C(52)	41.15(18)
C(55)-Fe(3)-C(52)	69.15(19)
C(63)-Fe(3)-C(52)	157.7(2)
C(61)-Fe(3)-C(52)	106.6(2)
C(62)-Fe(3)-C(65)	67.1(3)
C(51)-Fe(3)-C(65)	106.4(2)
C(55)-Fe(3)-C(65)	122.1(2)
C(63)-Fe(3)-C(65)	68.2(3)
C(61)-Fe(3)-C(65)	39.9(3)
C(52)-Fe(3)-C(65)	122.5(3)
C(62)-Fe(3)-C(64)	66.7(3)
C(51)-Fe(3)-C(64)	123.6(2)
C(55)-Fe(3)-C(64)	108.3(2)
C(63)-Fe(3)-C(64)	40.3(3)

C(61)-Fe(3)-C(64)	67.3(3)
C(52)-Fe(3)-C(64)	159.5(3)
C(65)-Fe(3)-C(64)	40.4(3)
C(62)-Fe(3)-C(54)	125.6(2)
C(51)-Fe(3)-C(54)	68.37(19)
C(55)-Fe(3)-C(54)	40.40(19)
C(63)-Fe(3)-C(54)	109.4(3)
C(61)-Fe(3)-C(54)	160.7(2)
C(52)-Fe(3)-C(54)	68.0(2)
C(65)-Fe(3)-C(54)	158.6(3)
C(64)-Fe(3)-C(54)	124.0(3)
C(62)-Fe(3)-C(53)	109.5(2)
C(51)-Fe(3)-C(53)	68.36(19)
C(55)-Fe(3)-C(53)	68.2(2)
C(63)-Fe(3)-C(53)	123.3(2)
C(61)-Fe(3)-C(53)	124.1(2)
C(52)-Fe(3)-C(53)	40.4(2)
C(65)-Fe(3)-C(53)	159.2(3)
C(64)-Fe(3)-C(53)	159.1(3)
C(54)-Fe(3)-C(53)	40.1(2)
C(4)-O(1)-Mn(1)	125.3(3)
C(2)-O(2)-Mn(1)	125.7(3)
C(8)-O(3)-Mn(1)	125.7(3)
C(6)-O(4)-Mn(1)	127.0(3)
C(12)-O(5)-Mn(1)	124.3(3)
C(10)-O(6)-Mn(1)	125.8(3)
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(2)-C(2)-C(3)	124.1(4)
O(2)-C(2)-C(1)	115.4(4)
C(3)-C(2)-C(1)	120.4(4)
C(2)-C(3)-C(4)	124.3(4)
C(2)-C(3)-H(3)	117.9
C(4)-C(3)-H(3)	117.9

O(1)-C(4)-C(3)	124.8(4)
O(1)-C(4)-C(13)	116.0(4)
C(3)-C(4)-C(13)	119.2(4)
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(4)-C(6)-C(7)	121.4(4)
O(4)-C(6)-C(5)	117.9(4)
C(7)-C(6)-C(5)	120.7(4)
C(8)-C(7)-C(6)	126.1(4)
C(8)-C(7)-H(7)	117.0
C(6)-C(7)-H(7)	117.0
O(3)-C(8)-C(7)	124.5(4)
O(3)-C(8)-C(31)	115.9(4)
C(7)-C(8)-C(31)	119.6(4)
C(10)-C(9)-H(9A)	109.5
C(10)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(10)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
O(6)-C(10)-C(11)	123.9(4)
O(6)-C(10)-C(9)	116.3(4)
C(11)-C(10)-C(9)	119.8(4)
C(10)-C(11)-C(12)	124.3(4)
C(10)-C(11)-H(11)	117.9
C(12)-C(11)-H(11)	117.9
O(5)-C(12)-C(11)	124.6(4)
O(5)-C(12)-C(51)	117.1(4)
C(11)-C(12)-C(51)	118.2(4)
C(17)-C(13)-C(14)	107.5(4)
C(17)-C(13)-C(4)	124.0(4)
C(14)-C(13)-C(4)	128.2(4)
C(17)-C(13)-Fe(1)	70.4(3)
C(14)-C(13)-Fe(1)	69.1(3)

C(4)-C(13)-Fe(1)	121.2(3)
C(15)-C(14)-C(13)	107.7(5)
C(15)-C(14)-Fe(1)	70.7(3)
C(13)-C(14)-Fe(1)	69.3(3)
C(15)-C(14)-H(14)	126.2
C(13)-C(14)-H(14)	126.2
Fe(1)-C(14)-H(14)	125.4
C(14)-C(15)-C(16)	108.9(5)
C(14)-C(15)-Fe(1)	69.0(3)
C(16)-C(15)-Fe(1)	69.7(3)
C(14)-C(15)-H(15)	125.6
C(16)-C(15)-H(15)	125.6
Fe(1)-C(15)-H(15)	127.3
C(15)-C(16)-C(17)	108.0(5)
C(15)-C(16)-Fe(1)	69.8(3)
C(17)-C(16)-Fe(1)	69.9(3)
C(15)-C(16)-H(16)	126.0
C(17)-C(16)-H(16)	126.0
Fe(1)-C(16)-H(16)	125.8
C(16)-C(17)-C(13)	107.9(5)
C(16)-C(17)-Fe(1)	69.6(3)
C(13)-C(17)-Fe(1)	68.8(3)
C(16)-C(17)-H(17)	126.0
C(13)-C(17)-H(17)	126.0
Fe(1)-C(17)-H(17)	127.2
C(22)-C(21)-C(25)	108.1(5)
C(22)-C(21)-Fe(1)	69.9(3)
C(25)-C(21)-Fe(1)	69.5(3)
C(22)-C(21)-H(21)	126.0
C(25)-C(21)-H(21)	126.0
Fe(1)-C(21)-H(21)	126.3
C(21)-C(22)-C(23)	108.2(5)
C(21)-C(22)-Fe(1)	69.8(3)
C(23)-C(22)-Fe(1)	69.8(3)
C(21)-C(22)-H(22)	125.9
C(23)-C(22)-H(22)	125.9
Fe(1)-C(22)-H(22)	126.1
C(24)-C(23)-C(22)	108.0(5)

C(24)-C(23)-Fe(1)	69.1(3)
C(22)-C(23)-Fe(1)	69.7(3)
C(24)-C(23)-H(23)	126.0
C(22)-C(23)-H(23)	126.0
Fe(1)-C(23)-H(23)	126.8
C(25)-C(24)-C(23)	108.2(5)
C(25)-C(24)-Fe(1)	70.0(3)
C(23)-C(24)-Fe(1)	70.3(3)
C(25)-C(24)-H(24)	125.9
C(23)-C(24)-H(24)	125.9
Fe(1)-C(24)-H(24)	125.4
C(24)-C(25)-C(21)	107.6(5)
C(24)-C(25)-Fe(1)	69.3(3)
C(21)-C(25)-Fe(1)	69.7(3)
C(24)-C(25)-H(25)	126.2
C(21)-C(25)-H(25)	126.2
Fe(1)-C(25)-H(25)	126.4
C(35)-C(31)-C(32)	107.6(4)
C(35)-C(31)-C(8)	127.3(4)
C(32)-C(31)-C(8)	124.3(4)
C(35)-C(31)-Fe(2)	69.6(3)
C(32)-C(31)-Fe(2)	70.1(3)
C(8)-C(31)-Fe(2)	117.4(3)
C(33)-C(32)-C(31)	108.0(4)
C(33)-C(32)-Fe(2)	70.1(3)
C(31)-C(32)-Fe(2)	68.5(3)
C(33)-C(32)-H(32)	126.0
C(31)-C(32)-H(32)	126.0
Fe(2)-C(32)-H(32)	127.0
C(32)-C(33)-C(34)	107.8(4)
C(32)-C(33)-Fe(2)	69.4(3)
C(34)-C(33)-Fe(2)	69.3(3)
C(32)-C(33)-H(33)	126.1
C(34)-C(33)-H(33)	126.1
Fe(2)-C(33)-H(33)	126.7
C(35)-C(34)-C(33)	108.8(4)
C(35)-C(34)-Fe(2)	69.2(3)
C(33)-C(34)-Fe(2)	70.0(3)

C(35)-C(34)-H(34)	125.6
C(33)-C(34)-H(34)	125.6
Fe(2)-C(34)-H(34)	126.8
C(34)-C(35)-C(31)	107.8(4)
C(34)-C(35)-Fe(2)	70.2(3)
C(31)-C(35)-Fe(2)	69.0(3)
C(34)-C(35)-H(35)	126.1
C(31)-C(35)-H(35)	126.1
Fe(2)-C(35)-H(35)	126.3
C(42)-C(41)-C(45)	108.2(4)
C(42)-C(41)-Fe(2)	70.6(3)
C(45)-C(41)-Fe(2)	69.7(3)
C(42)-C(41)-H(41)	125.9
C(45)-C(41)-H(41)	125.9
Fe(2)-C(41)-H(41)	125.4
C(41)-C(42)-C(43)	108.0(4)
C(41)-C(42)-Fe(2)	69.0(3)
C(43)-C(42)-Fe(2)	69.9(3)
C(41)-C(42)-H(42)	126.0
C(43)-C(42)-H(42)	126.0
Fe(2)-C(42)-H(42)	126.7
C(42)-C(43)-C(44)	107.4(4)
C(42)-C(43)-Fe(2)	69.6(3)
C(44)-C(43)-Fe(2)	69.0(3)
C(42)-C(43)-H(43)	126.3
C(44)-C(43)-H(43)	126.3
Fe(2)-C(43)-H(43)	126.6
C(45)-C(44)-C(43)	108.4(4)
C(45)-C(44)-Fe(2)	69.7(3)
C(43)-C(44)-Fe(2)	70.3(3)
C(45)-C(44)-H(44)	125.8
C(43)-C(44)-H(44)	125.8
Fe(2)-C(44)-H(44)	125.8
C(44)-C(45)-C(41)	108.0(5)
C(44)-C(45)-Fe(2)	70.0(3)
C(41)-C(45)-Fe(2)	69.5(3)
C(44)-C(45)-H(45)	126.0
C(41)-C(45)-H(45)	126.0

Fe(2)-C(45)-H(45)	126.1
C(52)-C(51)-C(55)	107.5(4)
C(52)-C(51)-C(12)	124.8(4)
C(55)-C(51)-C(12)	127.5(4)
C(52)-C(51)-Fe(3)	69.8(3)
C(55)-C(51)-Fe(3)	69.4(3)
C(12)-C(51)-Fe(3)	122.0(3)
C(53)-C(52)-C(51)	107.9(4)
C(53)-C(52)-Fe(3)	70.9(3)
C(51)-C(52)-Fe(3)	69.1(3)
C(53)-C(52)-H(52)	126.1
C(51)-C(52)-H(52)	126.1
Fe(3)-C(52)-H(52)	125.6
C(54)-C(53)-C(52)	108.1(4)
C(54)-C(53)-Fe(3)	69.6(3)
C(52)-C(53)-Fe(3)	68.8(3)
C(54)-C(53)-H(53)	125.9
C(52)-C(53)-H(53)	125.9
Fe(3)-C(53)-H(53)	127.3
C(55)-C(54)-C(53)	108.9(5)
C(55)-C(54)-Fe(3)	68.8(3)
C(53)-C(54)-Fe(3)	70.4(3)
C(55)-C(54)-H(54)	125.6
C(53)-C(54)-H(54)	125.6
Fe(3)-C(54)-H(54)	126.8
C(54)-C(55)-C(51)	107.6(4)
C(54)-C(55)-Fe(3)	70.8(3)
C(51)-C(55)-Fe(3)	69.3(3)
C(54)-C(55)-H(55)	126.2
C(51)-C(55)-H(55)	126.2
Fe(3)-C(55)-H(55)	125.3
C(65)-C(61)-C(62)	107.3(7)
C(65)-C(61)-Fe(3)	70.3(4)
C(62)-C(61)-Fe(3)	69.4(4)
C(65)-C(61)-H(61)	126.3
C(62)-C(61)-H(61)	126.3
Fe(3)-C(61)-H(61)	125.5
C(63)-C(62)-C(61)	110.0(7)

C(63)-C(62)-Fe(3)	70.5(4)
C(61)-C(62)-Fe(3)	70.3(4)
C(63)-C(62)-H(62)	125.0
C(61)-C(62)-H(62)	125.0
Fe(3)-C(62)-H(62)	125.8
C(62)-C(63)-C(64)	106.5(7)
C(62)-C(63)-Fe(3)	69.6(4)
C(64)-C(63)-Fe(3)	70.2(4)
C(62)-C(63)-H(63)	126.8
C(64)-C(63)-H(63)	126.8
Fe(3)-C(63)-H(63)	125.0
C(63)-C(64)-C(65)	108.5(7)
C(63)-C(64)-Fe(3)	69.5(4)
C(65)-C(64)-Fe(3)	69.7(4)
C(63)-C(64)-H(64)	125.7
C(65)-C(64)-H(64)	125.7
Fe(3)-C(64)-H(64)	126.6
C(61)-C(65)-C(64)	107.7(7)
C(61)-C(65)-Fe(3)	69.8(4)
C(64)-C(65)-Fe(3)	69.9(4)
C(61)-C(65)-H(65)	126.1
C(64)-C(65)-H(65)	126.1
Fe(3)-C(65)-H(65)	125.7
C(72)-C(71)-C(74)	109.6(16)
C(72)-C(71)-C(73)#1	117.9(11)
C(74)-C(71)-C(73)#1	132.2(15)
C(73)-C(72)-C(71)	119.0(12)
C(73)-C(72)-H(72)	120.5
C(71)-C(72)-H(72)	120.5
C(72)-C(73)-C(71)#1	123.1(10)
C(72)-C(73)-H(73)	118.5
C(71)#1-C(73)-H(73)	118.5
C(71)-C(74)-H(74A)	109.5
C(71)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
C(71)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
H(74C)-C(74)-H(74B)	109.5

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table 4S. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **3b**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	16(1)	13(1)	15(1)	4(1)	4(1)	7(1)
Fe(1)	17(1)	25(1)	15(1)	3(1)	5(1)	5(1)
Fe(2)	23(1)	18(1)	22(1)	6(1)	7(1)	13(1)
Fe(3)	20(1)	24(1)	35(1)	17(1)	9(1)	10(1)
O(1)	24(2)	20(2)	22(2)	9(1)	8(1)	11(1)
O(2)	29(2)	22(2)	19(2)	5(1)	10(1)	12(2)
O(3)	19(2)	19(2)	22(2)	7(1)	5(1)	8(1)
O(4)	27(2)	23(2)	28(2)	11(2)	11(2)	16(2)
O(5)	23(2)	25(2)	19(2)	8(1)	8(1)	11(1)
O(6)	18(2)	21(2)	23(2)	5(1)	4(1)	7(1)
C(1)	33(3)	20(3)	31(3)	10(2)	9(2)	10(2)
C(2)	12(2)	15(2)	24(2)	1(2)	1(2)	2(2)
C(3)	24(2)	17(2)	22(2)	4(2)	9(2)	11(2)
C(4)	10(2)	19(2)	20(2)	2(2)	1(2)	3(2)
C(5)	36(3)	40(3)	52(4)	24(3)	20(3)	24(3)
C(6)	17(2)	33(3)	12(2)	-3(2)	4(2)	16(2)
C(7)	19(2)	20(2)	23(2)	7(2)	7(2)	10(2)
C(8)	22(2)	19(2)	12(2)	3(2)	6(2)	10(2)
C(9)	23(3)	27(3)	36(3)	13(2)	9(2)	7(2)
C(10)	23(2)	14(2)	21(2)	4(2)	4(2)	12(2)
C(11)	23(2)	17(2)	18(2)	5(2)	6(2)	9(2)
C(12)	21(2)	14(2)	17(2)	5(2)	2(2)	10(2)
C(13)	15(2)	26(3)	18(2)	3(2)	4(2)	6(2)
C(14)	20(2)	35(3)	26(3)	5(2)	7(2)	13(2)
C(15)	17(2)	46(3)	20(3)	-1(2)	8(2)	7(2)
C(16)	23(3)	41(3)	22(3)	7(2)	8(2)	0(2)
C(17)	16(2)	24(3)	24(3)	6(2)	3(2)	-2(2)
C(21)	25(3)	24(3)	34(3)	-4(2)	9(2)	-3(2)
C(22)	23(3)	36(3)	20(3)	7(2)	0(2)	-3(2)
C(23)	14(2)	26(3)	28(3)	9(2)	1(2)	3(2)
C(24)	23(3)	34(3)	27(3)	12(2)	10(2)	3(2)
C(25)	29(3)	30(3)	49(3)	20(3)	14(3)	9(2)
C(31)	23(2)	23(2)	16(2)	6(2)	9(2)	12(2)

C(32)	31(3)	22(2)	26(3)	11(2)	13(2)	15(2)
C(33)	53(3)	27(3)	37(3)	22(2)	26(3)	25(3)
C(34)	44(3)	40(3)	28(3)	19(3)	13(2)	31(3)
C(35)	26(3)	29(3)	16(2)	4(2)	3(2)	15(2)
C(41)	28(3)	24(3)	23(2)	12(2)	11(2)	14(2)
C(42)	25(2)	24(3)	18(2)	3(2)	6(2)	7(2)
C(43)	45(3)	25(3)	29(3)	9(2)	17(2)	20(2)
C(44)	34(3)	51(4)	36(3)	22(3)	19(3)	29(3)
C(45)	24(3)	31(3)	27(3)	8(2)	11(2)	6(2)
C(51)	21(2)	16(2)	24(2)	7(2)	8(2)	10(2)
C(52)	25(2)	29(3)	37(3)	20(2)	17(2)	17(2)
C(53)	25(3)	23(3)	58(4)	26(3)	18(3)	10(2)
C(54)	23(3)	21(3)	39(3)	7(2)	2(2)	6(2)
C(55)	21(2)	19(2)	24(3)	2(2)	5(2)	7(2)
C(61)	61(2)	47(2)	81(2)	43(2)	30(2)	37(2)
C(62)	61(2)	47(2)	81(2)	43(2)	30(2)	37(2)
C(63)	61(2)	47(2)	81(2)	43(2)	30(2)	37(2)
C(64)	61(2)	47(2)	81(2)	43(2)	30(2)	37(2)
C(65)	61(2)	47(2)	81(2)	43(2)	30(2)	37(2)
C(71)	105(9)	118(9)	25(4)	10(5)	23(5)	47(8)
C(72)	141(11)	111(9)	30(5)	9(5)	39(6)	58(8)
C(73)	103(7)	62(6)	30(4)	7(4)	21(5)	22(6)
C(74)	103(17)	124(18)	27(9)	-1(10)	18(10)	-36(14)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3b**.

	x	y	z	U(eq)
H(1A)	8564	4221	4992	45
H(1B)	8978	5306	5966	45
H(1C)	7382	4387	5391	45
H(3)	8320	4432	3501	26
H(5A)	1472	3789	2032	59
H(5B)	2618	3298	1953	59
H(5C)	2454	3717	3014	59
H(7)	2080	5468	2042	26
H(9A)	5734	7772	7297	45
H(9B)	4313	7387	6310	45
H(9C)	4899	6518	6499	45
H(11)	7802	8651	7205	25
H(14)	8930	3989	2141	35
H(15)	9036	3879	457	40
H(16)	8160	5204	-18	41
H(17)	7622	6224	1427	32
H(21)	5660	2030	-787	43
H(22)	4770	3394	-1142	40
H(23)	4270	4327	359	32
H(24)	4907	3568	1665	36
H(25)	5733	2124	950	43
H(32)	5155	9025	3181	29
H(33)	3404	9824	2639	39
H(34)	953	8271	1582	40
H(35)	1157	6517	1483	31
H(41)	3341	7274	4543	29
H(42)	4569	9324	5313	30
H(43)	2710	10035	4760	38
H(44)	330	8400	3653	42
H(45)	717	6707	3537	35
H(52)	10556	9632	5505	31
H(53)	12735	11209	6996	39
H(54)	12304	11485	8605	39

H(55)	9863	10098	8139	29
H(61)	11695	7838	5822	66
H(62)	13947	9322	7275	66
H(63)	13637	9684	8919	66
H(64)	11176	8338	8490	66
H(65)	9963	7222	6569	66
H(72)	2080	1568	615	117
H(73)	-100	1632	137	88
H(74A)	2877	-421	856	175
H(74C)	3359	836	1069	175
H(74B)	2923	-58	-52	175

Table 6S. Torsion angles [°] for **3b**.

Mn(1)-O(2)-C(2)-C(3)	16.8(6)
Mn(1)-O(2)-C(2)-C(1)	-164.5(3)
O(2)-C(2)-C(3)-C(4)	4.8(7)
C(1)-C(2)-C(3)-C(4)	-173.8(4)
Mn(1)-O(1)-C(4)-C(3)	-17.5(6)
Mn(1)-O(1)-C(4)-C(13)	162.9(3)
C(2)-C(3)-C(4)-O(1)	-4.5(7)
C(2)-C(3)-C(4)-C(13)	175.1(4)
Mn(1)-O(4)-C(6)-C(7)	21.3(6)
Mn(1)-O(4)-C(6)-C(5)	-160.4(3)
O(4)-C(6)-C(7)-C(8)	-2.4(7)
C(5)-C(6)-C(7)-C(8)	179.3(5)
Mn(1)-O(3)-C(8)-C(7)	-20.2(6)
Mn(1)-O(3)-C(8)-C(31)	158.9(3)
C(6)-C(7)-C(8)-O(3)	2.0(7)
C(6)-C(7)-C(8)-C(31)	-177.1(4)
Mn(1)-O(6)-C(10)-C(11)	18.9(6)
Mn(1)-O(6)-C(10)-C(9)	-161.5(3)
O(6)-C(10)-C(11)-C(12)	4.5(7)
C(9)-C(10)-C(11)-C(12)	-175.0(4)
Mn(1)-O(5)-C(12)-C(11)	-20.0(6)
Mn(1)-O(5)-C(12)-C(51)	162.9(3)
C(10)-C(11)-C(12)-O(5)	-3.6(7)
C(10)-C(11)-C(12)-C(51)	173.5(4)
O(1)-C(4)-C(13)-C(17)	-5.3(6)
C(3)-C(4)-C(13)-C(17)	175.0(4)
O(1)-C(4)-C(13)-C(14)	-178.5(4)
C(3)-C(4)-C(13)-C(14)	1.9(7)
O(1)-C(4)-C(13)-Fe(1)	-91.6(5)
C(3)-C(4)-C(13)-Fe(1)	88.8(5)
C(17)-C(13)-C(14)-C(15)	0.4(5)
C(4)-C(13)-C(14)-C(15)	174.5(4)
Fe(1)-C(13)-C(14)-C(15)	60.6(3)
C(17)-C(13)-C(14)-Fe(1)	-60.2(3)
C(4)-C(13)-C(14)-Fe(1)	113.9(5)
C(13)-C(14)-C(15)-C(16)	-1.3(6)

Fe(1)-C(14)-C(15)-C(16)	58.4(3)
C(13)-C(14)-C(15)-Fe(1)	-59.7(3)
C(14)-C(15)-C(16)-C(17)	1.7(6)
Fe(1)-C(15)-C(16)-C(17)	59.7(3)
C(14)-C(15)-C(16)-Fe(1)	-58.0(3)
C(15)-C(16)-C(17)-C(13)	-1.5(5)
Fe(1)-C(16)-C(17)-C(13)	58.2(3)
C(15)-C(16)-C(17)-Fe(1)	-59.7(3)
C(14)-C(13)-C(17)-C(16)	0.7(5)
C(4)-C(13)-C(17)-C(16)	-173.7(4)
Fe(1)-C(13)-C(17)-C(16)	-58.8(3)
C(14)-C(13)-C(17)-Fe(1)	59.4(3)
C(4)-C(13)-C(17)-Fe(1)	-115.0(4)
C(25)-C(21)-C(22)-C(23)	-0.2(6)
Fe(1)-C(21)-C(22)-C(23)	-59.4(3)
C(25)-C(21)-C(22)-Fe(1)	59.2(3)
C(21)-C(22)-C(23)-C(24)	0.7(5)
Fe(1)-C(22)-C(23)-C(24)	-58.7(3)
C(21)-C(22)-C(23)-Fe(1)	59.4(3)
C(22)-C(23)-C(24)-C(25)	-1.0(5)
Fe(1)-C(23)-C(24)-C(25)	-60.0(3)
C(22)-C(23)-C(24)-Fe(1)	59.0(3)
C(23)-C(24)-C(25)-C(21)	0.8(6)
Fe(1)-C(24)-C(25)-C(21)	-59.3(3)
C(23)-C(24)-C(25)-Fe(1)	60.2(3)
C(22)-C(21)-C(25)-C(24)	-0.3(6)
Fe(1)-C(21)-C(25)-C(24)	59.1(3)
C(22)-C(21)-C(25)-Fe(1)	-59.4(3)
O(3)-C(8)-C(31)-C(35)	179.5(4)
C(7)-C(8)-C(31)-C(35)	-1.3(7)
O(3)-C(8)-C(31)-C(32)	-12.4(6)
C(7)-C(8)-C(31)-C(32)	166.8(4)
O(3)-C(8)-C(31)-Fe(2)	-96.1(4)
C(7)-C(8)-C(31)-Fe(2)	83.1(5)
C(35)-C(31)-C(32)-C(33)	0.7(5)
C(8)-C(31)-C(32)-C(33)	-169.4(4)
Fe(2)-C(31)-C(32)-C(33)	-59.1(3)
C(35)-C(31)-C(32)-Fe(2)	59.8(3)

C(8)-C(31)-C(32)-Fe(2)	-110.3(4)
C(31)-C(32)-C(33)-C(34)	-0.7(5)
Fe(2)-C(32)-C(33)-C(34)	-58.9(3)
C(31)-C(32)-C(33)-Fe(2)	58.1(3)
C(32)-C(33)-C(34)-C(35)	0.5(6)
Fe(2)-C(33)-C(34)-C(35)	-58.4(3)
C(32)-C(33)-C(34)-Fe(2)	58.9(3)
C(33)-C(34)-C(35)-C(31)	0.0(5)
Fe(2)-C(34)-C(35)-C(31)	-58.9(3)
C(33)-C(34)-C(35)-Fe(2)	58.9(4)
C(32)-C(31)-C(35)-C(34)	-0.4(5)
C(8)-C(31)-C(35)-C(34)	169.3(4)
Fe(2)-C(31)-C(35)-C(34)	59.7(3)
C(32)-C(31)-C(35)-Fe(2)	-60.1(3)
C(8)-C(31)-C(35)-Fe(2)	109.6(4)
C(45)-C(41)-C(42)-C(43)	-0.6(5)
Fe(2)-C(41)-C(42)-C(43)	59.2(3)
C(45)-C(41)-C(42)-Fe(2)	-59.8(3)
C(41)-C(42)-C(43)-C(44)	0.2(6)
Fe(2)-C(42)-C(43)-C(44)	58.9(3)
C(41)-C(42)-C(43)-Fe(2)	-58.7(3)
C(42)-C(43)-C(44)-C(45)	0.2(6)
Fe(2)-C(43)-C(44)-C(45)	59.5(4)
C(42)-C(43)-C(44)-Fe(2)	-59.3(3)
C(43)-C(44)-C(45)-C(41)	-0.6(6)
Fe(2)-C(44)-C(45)-C(41)	59.3(3)
C(43)-C(44)-C(45)-Fe(2)	-59.9(4)
C(42)-C(41)-C(45)-C(44)	0.7(5)
Fe(2)-C(41)-C(45)-C(44)	-59.6(3)
C(42)-C(41)-C(45)-Fe(2)	60.3(3)
O(5)-C(12)-C(51)-C(52)	-5.4(6)
C(11)-C(12)-C(51)-C(52)	177.2(4)
O(5)-C(12)-C(51)-C(55)	-179.3(4)
C(11)-C(12)-C(51)-C(55)	3.3(7)
O(5)-C(12)-C(51)-Fe(3)	-91.9(4)
C(11)-C(12)-C(51)-Fe(3)	90.8(5)
C(55)-C(51)-C(52)-C(53)	-1.2(5)
C(12)-C(51)-C(52)-C(53)	-176.1(4)

Fe(3)-C(51)-C(52)-C(53)	-60.5(3)
C(55)-C(51)-C(52)-Fe(3)	59.3(3)
C(12)-C(51)-C(52)-Fe(3)	-115.6(4)
C(51)-C(52)-C(53)-C(54)	0.8(5)
Fe(3)-C(52)-C(53)-C(54)	-58.6(3)
C(51)-C(52)-C(53)-Fe(3)	59.4(3)
C(52)-C(53)-C(54)-C(55)	-0.1(6)
Fe(3)-C(53)-C(54)-C(55)	-58.2(4)
C(52)-C(53)-C(54)-Fe(3)	58.1(3)
C(53)-C(54)-C(55)-C(51)	-0.6(6)
Fe(3)-C(54)-C(55)-C(51)	-59.8(3)
C(53)-C(54)-C(55)-Fe(3)	59.1(4)
C(52)-C(51)-C(55)-C(54)	1.1(5)
C(12)-C(51)-C(55)-C(54)	175.9(4)
Fe(3)-C(51)-C(55)-C(54)	60.7(3)
C(52)-C(51)-C(55)-Fe(3)	-59.6(3)
C(12)-C(51)-C(55)-Fe(3)	115.2(4)
C(65)-C(61)-C(62)-C(63)	-0.9(7)
Fe(3)-C(61)-C(62)-C(63)	59.5(4)
C(65)-C(61)-C(62)-Fe(3)	-60.4(4)
C(61)-C(62)-C(63)-C(64)	1.5(7)
Fe(3)-C(62)-C(63)-C(64)	60.9(4)
C(61)-C(62)-C(63)-Fe(3)	-59.4(4)
C(62)-C(63)-C(64)-C(65)	-1.5(7)
Fe(3)-C(63)-C(64)-C(65)	59.0(4)
C(62)-C(63)-C(64)-Fe(3)	-60.5(4)
C(62)-C(61)-C(65)-C(64)	-0.1(7)
Fe(3)-C(61)-C(65)-C(64)	-59.9(4)
C(62)-C(61)-C(65)-Fe(3)	59.8(4)
C(63)-C(64)-C(65)-C(61)	1.0(7)
Fe(3)-C(64)-C(65)-C(61)	59.8(4)
C(63)-C(64)-C(65)-Fe(3)	-58.8(4)
C(74)-C(71)-C(72)-C(73)	175.8(10)
C(73)#1-C(71)-C(72)-C(73)	0.8(13)
C(71)-C(72)-C(73)-C(71)#1	-0.8(14)

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