Tables of crystallographic data, atomic coordinates, interatomic distances and angles, anisotropic displacement parameters, and hydrogen atom coordinates for (η^5-$C_{13}H_9$)$Mn(CO)_3$, 1.

Table 1. Crystal data and structure refinement for $(\eta^5\text{-}C_{13}H_9)Mn(CO)_3$.

Identification code	ad000744
Empirical formula	C16 H9 Mn O3
Formula weight	304.17
Temperature	173(2) K
Wavelength	0.71073 Å
Diffractometer used	Bruker AXS P4/SMART 1000
Detector distance	4 cm
Monochromator used	Graphite
Crystal system	Orthorhombic
Colour and habit	Orange, irregular
Crystal size	0.125 x 0.125 x 0.325 mm^3
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 8.6242(4) Å α = 90°
	b = 10.2424(4) Å β = 90°
	c = 29.6826(13) Å γ = 90°
Volume	2621.9(2) $Å^3$
Z	8
Density (calculated)	1.541 Mg/m^3
Absorption coefficient	1.009 mm^{-1}
F(000)	1232
Theta range	1.37 to 32.50°
Completeness to theta = 32.50°	99.5 %
Scan type	ω and ϕ
Scan range	0.3°
Exposure time	30s
Index ranges	$-12 \le h \le 12$, $-15 \le k \le 15$, $-41 \le l \le 44$

Standard reflections	all frames
Crystal stability	no decay
Reflections collected	29206
Independent reflections	9163 [R(int) = 0.0250]
System used	SHELXTL 5.1
Solution	Direct methods
Hydrogen atoms	Found, refined isotropically
Absorption correction	SADABS
Max./Min. transmission	1.000/0.844
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9163 / 0 / 433
Goodness-of-fit on F^2	0.919
Final R indices [I>2sigma(I)]	R1 = 0.0290, wR2 = 0.0578
R indices (all data)	R1 = 0.0415, wR2 = 0.0600
Absolute structure parameter	-0.002 (9)
Largest/mean shift/esd	0.001/0.000
Largest diff. peak and hole	0.524 and -0.183 e.Å^{-3}

$wR2 = (\Sigma[w(F_o^2-F_c^2)^2/\Sigma[wF_o^4])^{1/2}$

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$

$Weight = 1 / [\sigma^2(F_o^2) + (0.0304 * P)^2]$

where $P = (\max(F_o^2, 0) + 2 * F_c^2)/3$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (η^5-$C_{13}H_9$)Mn(CO)$_3$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(1)	5029(1)	3018(1)	1464(1)	26(1)
C(1A)	5842(2)	1526(1)	1935(1)	28(1)
C(1)	5354(2)	1381(2)	2392(1)	36(1)
C(2)	6105(2)	2053(2)	2717(1)	44(1)
C(3)	7350(2)	2909(2)	2616(1)	42(1)
C(4)	7842(2)	3097(2)	2186(1)	33(1)
C(4A)	7096(2)	2399(2)	1835(1)	27(1)
C(5A)	7390(2)	2297(1)	1353(1)	28(1)
C(5)	8530(2)	2880(2)	1071(1)	35(1)
C(6)	8563(2)	2531(2)	627(1)	43(1)
C(7)	7486(3)	1627(2)	449(1)	45(1)
C(8)	6368(2)	1063(2)	705(1)	39(1)
C(8A)	6306(2)	1379(2)	1175(1)	30(1)
C(9)	5293(2)	966(1)	1526(1)	31(1)
C(10)	5652(2)	4697(2)	1440(1)	34(1)
C(11)	3825(2)	3133(2)	978(1)	38(1)
C(12)	3382(2)	3328(2)	1811(1)	40(1)
O(10)	6113(2)	5742(1)	1426(1)	50(1)
O(11)	3028(2)	3167(2)	670(1)	63(1)
O(12)	2297(2)	3477(2)	2027(1)	67(1)
Mn(2)	552(1)	7581(1)	1016(1)	27(1)
C(21A)	-915(2)	8597(2)	529(1)	29(1)
C(21)	-1024(2)	8297(2)	60(1)	37(1)
C(22)	-51(3)	8891(2)	-232(1)	41(1)
C(23)	1117(2)	9768(2)	-84(1)	40(1)
C(24)	1296(2)	10058(2)	358(1)	33(1)

C(24A)	271(2)	9477(1)	675(1)	27(1)
C(25A)	85(2)	9660(1)	1157(1)	27(1)
C(25)	854(2)	10485(2)	1470(1)	32(1)
C(26)	344(2)	10509(2)	1902(1)	39(1)
C(27)	-916(2)	9724(2)	2044(1)	42(1)
C(28)	-1676(2)	8919(2)	1759(1)	38(1)
C(29)	-1769(2)	8169(2)	915(1)	33(1)
C(30)	2604(2)	7792(2)	1084(1)	32(1)
C(31)	329(2)	6496(2)	1485(1)	37(1)
C(32)	669(2)	6211(2)	642(1)	35(1)
C(28A)	-1215(2)	8883(2)	1294(1)	30(1)
O(30)	3907(1)	7993(1)	1129(1)	45(1)
O(31)	159(2)	5808(1)	1785(1)	57(1)
O(32)	689(2)	5346(1)	397(1)	52(1)

Table 3. Bond lengths [Å] and angles [°] for $(\eta^5\text{-}C_{13}H_9)Mn(CO)_3$.

Mn(1)-C(12)	1.7816(19)
Mn(1)-C(11)	1.7831(17)
Mn(1)-C(10)	1.8025(17)
Mn(1)-C(9)	2.1223(15)
Mn(1)-C(8A)	2.1838(15)
Mn(1)-C(1A)	2.1852(15)
Mn(1)-C(4A)	2.1881(14)
Mn(1)-C(5A)	2.1906(15)
C(1A)-C(9)	1.424(2)
C(1A)-C(1)	1.429(2)
C(1A)-C(4A)	1.435(2)
C(1)-C(2)	1.350(2)
C(2)-C(3)	1.418(3)
C(3)-C(4)	1.360(2)
C(4)-C(4A)	1.418(2)
C(4A)-C(5A)	1.455(2)
C(5A)-C(5)	1.422(2)
C(5A)-C(8A)	1.428(2)
C(5)-C(6)	1.366(2)
C(6)-C(7)	1.413(3)
C(7)-C(8)	1.355(3)
C(8)-C(8A)	1.435(2)
C(8A)-C(9)	1.424(2)
C(10)-O(10)	1.143(2)
C(11)-O(11)	1.144(2)
C(12)-O(12)	1.146(2)
Mn(2)-C(31)	1.7912(17)
Mn(2)-C(32)	1.7923(17)
Mn(2)-C(30)	1.7948(16)

Mn(2)-C(29)	2.1121(16)
Mn(2)-C(28A)	2.1860(16)
Mn(2)-C(21A)	2.1861(15)
Mn(2)-C(24A)	2.2044(14)
Mn(2)-C(25A)	2.2073(14)
C(21A)-C(21)	1.428(2)
C(21A)-C(24A)	1.430(2)
C(21A)-C(29)	1.431(2)
C(21)-C(22)	1.351(3)
C(22)-C(23)	1.418(3)
C(23)-C(24)	1.354(3)
C(24)-C(24A)	1.421(2)
C(24A)-C(25A)	1.453(2)
C(25A)-C(25)	1.419(2)
C(25A)-C(28A)	1.434(2)
C(25)-C(26)	1.357(2)
C(26)-C(27)	1.415(3)
C(27)-C(28)	1.351(3)
C(28)-C(28A)	1.435(2)
C(29)-C(28A)	1.426(2)
C(30)-O(30)	1.150(2)
C(31)-O(31)	1.144(2)
C(32)-O(32)	1.148(2)

C(12)-Mn(1)-C(11)	89.51(9)
C(12)-Mn(1)-C(10)	95.20(8)
C(11)-Mn(1)-C(10)	94.48(8)
C(12)-Mn(1)-C(9)	102.25(7)
C(11)-Mn(1)-C(9)	101.37(7)
C(10)-Mn(1)-C(9)	156.39(7)
C(12)-Mn(1)-C(8A)	139.97(7)

C(11)-Mn(1)-C(8A)	91.45(7)
C(10)-Mn(1)-C(8A)	124.57(7)
C(9)-Mn(1)-C(8A)	38.58(6)
C(12)-Mn(1)-C(1A)	90.69(7)
C(11)-Mn(1)-C(1A)	138.63(7)
C(10)-Mn(1)-C(1A)	126.66(7)
C(9)-Mn(1)-C(1A)	38.56(6)
C(8A)-Mn(1)-C(1A)	63.37(6)
C(12)-Mn(1)-C(4A)	114.30(7)
C(11)-Mn(1)-C(4A)	154.21(7)
C(10)-Mn(1)-C(4A)	93.08(7)
C(9)-Mn(1)-C(4A)	65.33(6)
C(8A)-Mn(1)-C(4A)	64.16(6)
C(1A)-Mn(1)-C(4A)	38.30(6)
C(12)-Mn(1)-C(5A)	152.62(7)
C(11)-Mn(1)-C(5A)	116.17(7)
C(10)-Mn(1)-C(5A)	92.20(7)
C(9)-Mn(1)-C(5A)	65.15(6)
C(8A)-Mn(1)-C(5A)	38.11(6)
C(1A)-Mn(1)-C(5A)	64.06(6)
C(4A)-Mn(1)-C(5A)	38.82(5)
C(9)-C(1A)-C(1)	132.03(14)
C(9)-C(1A)-C(4A)	109.03(13)
C(1)-C(1A)-C(4A)	118.93(14)
C(9)-C(1A)-Mn(1)	68.33(8)
C(1)-C(1A)-Mn(1)	125.80(11)
C(4A)-C(1A)-Mn(1)	70.96(8)
C(2)-C(1)-C(1A)	118.92(16)
C(1)-C(2)-C(3)	121.93(16)
C(4)-C(3)-C(2)	121.41(16)
C(3)-C(4)-C(4A)	118.55(15)

C(4)-C(4A)-C(1A)	120.24(13)
C(4)-C(4A)-C(5A)	132.80(14)
C(1A)-C(4A)-C(5A)	106.85(13)
C(4)-C(4A)-Mn(1)	126.35(11)
C(1A)-C(4A)-Mn(1)	70.74(8)
C(5A)-C(4A)-Mn(1)	70.68(8)
C(5)-C(5A)-C(8A)	120.73(14)
C(5)-C(5A)-C(4A)	131.95(14)
C(8A)-C(5A)-C(4A)	107.26(13)
C(5)-C(5A)-Mn(1)	126.15(10)
C(8A)-C(5A)-Mn(1)	70.69(8)
C(4A)-C(5A)-Mn(1)	70.49(8)
C(6)-C(5)-C(5A)	118.24(17)
C(5)-C(6)-C(7)	121.12(17)
C(8)-C(7)-C(6)	122.57(17)
C(7)-C(8)-C(8A)	118.37(18)
C(9)-C(8A)-C(5A)	109.09(13)
C(9)-C(8A)-C(8)	131.94(16)
C(5A)-C(8A)-C(8)	118.94(16)
C(9)-C(8A)-Mn(1)	68.37(9)
C(5A)-C(8A)-Mn(1)	71.21(8)
C(8)-C(8A)-Mn(1)	125.10(11)
C(1A)-C(9)-C(8A)	107.42(13)
C(1A)-C(9)-Mn(1)	73.11(8)
C(8A)-C(9)-Mn(1)	73.05(9)
O(10)-C(10)-Mn(1)	176.94(16)
O(11)-C(11)-Mn(1)	177.59(18)
O(12)-C(12)-Mn(1)	177.05(17)
C(31)-Mn(2)-C(32)	90.10(8)
C(31)-Mn(2)-C(30)	95.35(7)
C(32)-Mn(2)-C(30)	96.21(7)

C(31)-Mn(2)-C(29)	100.75(7)
C(32)-Mn(2)-C(29)	100.84(7)
C(30)-Mn(2)-C(29)	156.43(7)
C(31)-Mn(2)-C(28A)	90.62(7)
C(32)-Mn(2)-C(28A)	138.65(7)
C(30)-Mn(2)-C(28A)	124.85(6)
C(29)-Mn(2)-C(28A)	38.71(6)
C(31)-Mn(2)-C(21A)	138.41(7)
C(32)-Mn(2)-C(21A)	89.72(7)
C(30)-Mn(2)-C(21A)	126.00(6)
C(29)-Mn(2)-C(21A)	38.84(6)
C(28A)-Mn(2)-C(21A)	63.65(6)
C(31)-Mn(2)-C(24A)	153.19(7)
C(32)-Mn(2)-C(24A)	114.24(6)
C(30)-Mn(2)-C(24A)	93.09(6)
C(29)-Mn(2)-C(24A)	65.10(6)
C(28A)-Mn(2)-C(24A)	63.88(6)
C(21A)-Mn(2)-C(24A)	38.02(5)
C(31)-Mn(2)-C(25A)	115.62(7)
C(32)-Mn(2)-C(25A)	151.97(7)
C(30)-Mn(2)-C(25A)	92.44(6)
C(29)-Mn(2)-C(25A)	65.10(6)
C(28A)-Mn(2)-C(25A)	38.09(6)
C(21A)-Mn(2)-C(25A)	63.90(6)
C(24A)-Mn(2)-C(25A)	38.46(5)
C(21)-C(21A)-C(24A)	118.55(14)
C(21)-C(21A)-C(29)	132.83(15)
C(24A)-C(21A)-C(29)	108.62(13)
C(21)-C(21A)-Mn(2)	125.52(11)
C(24A)-C(21A)-Mn(2)	71.68(8)
C(29)-C(21A)-Mn(2)	67.79(9)

C(22)-C(21)-C(21A)	119.11(16)
C(21)-C(22)-C(23)	121.90(16)
C(24)-C(23)-C(22)	121.29(17)
C(23)-C(24)-C(24A)	118.56(16)
C(24)-C(24A)-C(21A)	120.55(14)
C(24)-C(24A)-C(25A)	131.82(15)
C(21A)-C(24A)-C(25A)	107.49(13)
C(24)-C(24A)-Mn(2)	127.24(11)
C(21A)-C(24A)-Mn(2)	70.30(8)
C(25A)-C(24A)-Mn(2)	70.88(8)
C(25)-C(25A)-C(28A)	120.63(14)
C(25)-C(25A)-C(24A)	132.04(15)
C(28A)-C(25A)-C(24A)	107.16(13)
C(25)-C(25A)-Mn(2)	127.76(11)
C(28A)-C(25A)-Mn(2)	70.15(8)
C(24A)-C(25A)-Mn(2)	70.66(8)
C(26)-C(25)-C(25A)	118.56(16)
C(25)-C(26)-C(27)	121.26(17)
C(28)-C(27)-C(26)	122.26(17)
C(27)-C(28)-C(28A)	118.83(17)
C(28A)-C(29)-C(21A)	107.61(13)
C(28A)-C(29)-Mn(2)	73.44(9)
C(21A)-C(29)-Mn(2)	73.37(9)
O(30)-C(30)-Mn(2)	176.58(14)
O(31)-C(31)-Mn(2)	178.78(17)
O(32)-C(32)-Mn(2)	177.39(17)
C(29)-C(28A)-C(25A)	108.80(14)
C(29)-C(28A)-C(28)	132.78(16)
C(25A)-C(28A)-C(28)	118.40(16)
C(29)-C(28A)-Mn(2)	67.84(9)
C(25A)-C(28A)-Mn(2)	71.76(8)

C(28)-C(28A)-Mn(2) 124.82(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $(\eta^5\text{-}C_{13}H_9)Mn(CO)_3$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(1)	30(1)	26(1)	24(1)	0(1)	-1(1)	4(1)
C(1A)	29(1)	26(1)	29(1)	4(1)	-3(1)	0(1)
C(1)	40(1)	38(1)	31(1)	8(1)	2(1)	-7(1)
C(2)	53(1)	54(1)	24(1)	7(1)	1(1)	-8(1)
C(3)	52(1)	45(1)	27(1)	-1(1)	-10(1)	-8(1)
C(4)	33(1)	33(1)	34(1)	2(1)	-6(1)	-6(1)
C(4A)	29(1)	27(1)	25(1)	3(1)	-2(1)	2(1)
C(5A)	32(1)	25(1)	27(1)	3(1)	0(1)	5(1)
C(5)	37(1)	31(1)	38(1)	6(1)	6(1)	5(1)
C(6)	52(1)	40(1)	36(1)	8(1)	14(1)	16(1)
C(7)	65(1)	43(1)	28(1)	-2(1)	4(1)	21(1)
C(8)	52(1)	35(1)	29(1)	-7(1)	-8(1)	12(1)
C(8A)	35(1)	27(1)	29(1)	-2(1)	-4(1)	8(1)
C(9)	33(1)	26(1)	33(1)	-1(1)	-5(1)	-1(1)
C(10)	39(1)	32(1)	30(1)	1(1)	3(1)	9(1)
C(11)	43(1)	35(1)	36(1)	2(1)	-4(1)	7(1)
C(12)	44(1)	33(1)	43(1)	-4(1)	4(1)	6(1)
O(10)	61(1)	29(1)	61(1)	3(1)	8(1)	1(1)
O(11)	74(1)	64(1)	50(1)	7(1)	-32(1)	4(1)
O(12)	61(1)	63(1)	76(1)	-10(1)	35(1)	8(1)
Mn(2)	29(1)	24(1)	29(1)	3(1)	0(1)	2(1)
C(21A)	28(1)	27(1)	33(1)	5(1)	-3(1)	1(1)
C(21)	42(1)	33(1)	35(1)	0(1)	-10(1)	-2(1)
C(22)	55(1)	41(1)	29(1)	1(1)	-5(1)	2(1)
C(23)	48(1)	39(1)	34(1)	7(1)	7(1)	-2(1)
C(24)	36(1)	29(1)	35(1)	3(1)	3(1)	-3(1)

C(24A)	28(1)	25(1)	27(1)	4(1)	0(1)	2(1)
C(25A)	27(1)	26(1)	29(1)	3(1)	2(1)	4(1)
C(25)	34(1)	29(1)	34(1)	1(1)	-2(1)	5(1)
C(26)	46(1)	38(1)	31(1)	-4(1)	-4(1)	13(1)
C(27)	52(1)	45(1)	30(1)	5(1)	8(1)	18(1)
C(28)	37(1)	38(1)	40(1)	12(1)	13(1)	9(1)
C(29)	26(1)	30(1)	42(1)	6(1)	0(1)	-3(1)
C(30)	37(1)	31(1)	28(1)	-3(1)	0(1)	6(1)
C(31)	40(1)	32(1)	40(1)	4(1)	-1(1)	2(1)
C(32)	34(1)	31(1)	40(1)	3(1)	0(1)	1(1)
C(28A)	30(1)	28(1)	33(1)	7(1)	4(1)	5(1)
O(30)	32(1)	51(1)	51(1)	-9(1)	-4(1)	4(1)
O(31)	73(1)	48(1)	51(1)	25(1)	-4(1)	-2(1)
O(32)	59(1)	36(1)	60(1)	-14(1)	-1(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $(\eta^5\text{-}C_{13}H_9)Mn(CO)_3$.

	x	y	z	U(eq)
H(1)	4610(20)	820(20)	2477(6)	42(5)
H(2)	5790(30)	1900(20)	3021(8)	67(7)
H(3)	7800(20)	3304(17)	2839(6)	32(5)
H(4)	8700(20)	3679(18)	2132(6)	32(5)
H(5)	9240(20)	3481(18)	1185(5)	30(4)
H(6)	9400(20)	2850(18)	441(6)	39(5)
H(7)	7580(20)	1349(18)	119(6)	36(5)
H(8)	5670(20)	457(19)	586(6)	42(5)
H(9)	4470(20)	387(19)	1512(7)	47(5)
H(21)	-1690(20)	7730(20)	-57(6)	45(5)
H(22)	-100(20)	8733(19)	-541(7)	49(5)
H(23)	1790(30)	10130(20)	-304(7)	53(6)
H(24)	2040(20)	10666(19)	461(6)	39(5)
H(25)	1650(20)	11022(17)	1366(6)	32(5)
H(26)	810(20)	11050(20)	2117(6)	45(5)
H(27)	-1300(30)	9820(20)	2349(8)	60(7)
H(28)	-2490(20)	8403(18)	1844(6)	31(5)
H(29)	-2630(20)	7580(20)	897(6)	42(5)

Tables of crystallographic data, atomic coordinates, interatomic distances and angles, anisotropic displacement parameters, and hydrogen atom coordinates for (η^1-$C_{13}H_9$)$Mn(CO)_5$, 2.

Table 1. Crystal data and structure refinement for C_{18} H_9 Mn O_5.

Identification code	ad0522	
Empirical formula	C18 H9 Mn O5	
Formula weight	360.19	
Temperature	295(1) K	
Wavelength	0.71073 Å	
Monochromator used	Graphite	
Diffractometer used	Bruker AXS P4/SMART 1000	
Colour and habit	Yellow, irregular	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.2617(4) Å	α = 90°
	b = 25.2882(11) Å	β = 98.7440(10)°
	c = 6.8122(3) Å	γ = 90°
Volume	1576.95(12) $Å^3$	
Z	4	
Density (calculated)	1.517 Mg/m^3	
Absorption coefficient	0.861 mm^{-1}	
F(000)	728	
Crystal size	0.075 x 0.15 x 0.275 mm^3	
Theta range	2.22 to 32.50°	
Completeness to theta = 32.50°	98.5 %	
Scan type	ω and ϕ	
Scan range	0.3°	
Exposure time	30s	
Index ranges	$-13 \le h \le 13$, $-38 \le k \le 36$, $-9 \le l \le 10$	
Standard reflections	all frames	
Crystal stability	no decay	
Reflections collected	17344	

Independent reflections	5626 [R(int) = 0.0229]
System used	SHELXTL 5.1
Solution	Direct methods
Hydrogen atoms	Found, refined isotropically
Absorption correction	SADABS
Max./Min. transmission	0.9487/0.8468
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5626 / 0 / 253
Goodness-of-fit on F^2	0.803
Final R indices [I>2sigma(I)]	R1 = 0.0379, wR2 = 0.0805
R indices (all data)	R1 = 0.0822, wR2 = 0.0869
Largest/mean shift/esd	0.001/0.000
Largest diff. peak and hole	0.492 and -0.143 e.Å^{-3}

$wR2 = (\Sigma[w(F_o^2-F_c^2)^2/\Sigma[wF_o^4])^{1/2}$

$R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$

$Weight = 1 / [\sigma^2(F_o^2) + (0.0459 * P)^2$

where $P = (\max(F_o^2, 0) + 2 * F_c^2)/3$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C_{18} H_9 Mn O_5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn	7338(1)	529(1)	7369(1)	47(1)
C(1A)	8157(2)	1593(1)	9642(2)	43(1)
C(1)	9650(2)	1579(1)	10285(2)	55(1)
C(2)	10199(2)	1784(1)	12132(3)	64(1)
C(3)	9289(2)	2007(1)	13330(2)	63(1)
C(4)	7808(2)	2028(1)	12713(2)	55(1)
C(4A)	7237(2)	1822(1)	10859(2)	44(1)
C(5A)	5748(2)	1824(1)	9788(2)	44(1)
C(5)	4464(2)	2017(1)	10328(3)	57(1)
C(6)	3206(2)	1996(1)	8968(3)	67(1)
C(7)	3222(2)	1790(1)	7103(3)	68(1)
C(8)	4490(2)	1598(1)	6536(3)	57(1)
C(8A)	5774(2)	1605(1)	7891(2)	44(1)
C(9)	7275(2)	1411(1)	7736(2)	44(1)
C(10)	7402(2)	-186(1)	6984(3)	66(1)
C(11)	9163(2)	643(1)	6622(2)	59(1)
C(12)	8208(2)	450(1)	9993(2)	55(1)
C(13)	5505(2)	494(1)	8178(2)	51(1)
C(14)	6485(2)	657(1)	4780(2)	57(1)
O(10)	7449(2)	-630(1)	6766(3)	98(1)
O(11)	10262(2)	714(1)	6171(2)	87(1)
O(12)	8764(2)	379(1)	11567(2)	79(1)
O(13)	4391(1)	459(1)	8645(2)	70(1)
O(14)	5959(2)	735(1)	3185(2)	82(1)

Table 3. Bond lengths [Å] and angles [°] for C_{18} H_9 Mn O_5.

Mn-C(10)	1.8300(19)
Mn-C(14)	1.8485(18)
Mn-C(12)	1.8562(17)
Mn-C(11)	1.8605(19)
Mn-C(13)	1.8647(17)
Mn-C(9)	2.2472(15)
C(1A)-C(1)	1.385(2)
C(1A)-C(4A)	1.4012(19)
C(1A)-C(9)	1.4978(19)
C(1)-C(2)	1.384(2)
C(1)-H(1)	0.940(17)
C(2)-C(3)	1.380(3)
C(2)-H(2)	0.929(18)
C(3)-C(4)	1.373(2)
C(3)-H(3)	0.970(17)
C(4)-C(4A)	1.394(2)
C(4)-H(4)	0.950(16)
C(4A)-C(5A)	1.459(2)
C(5A)-C(5)	1.386(2)
C(5A)-C(8A)	1.4091(18)
C(5)-C(6)	1.375(2)
C(5)-H(5)	1.010(16)
C(6)-C(7)	1.376(3)
C(6)-H(6)	0.948(18)
C(7)-C(8)	1.379(3)
C(7)-H(7)	0.947(19)
C(8)-C(8A)	1.390(2)
C(8)-H(8)	0.915(16)
C(8A)-C(9)	1.492(2)

C(9)-H(9)	0.906(15)
C(10)-O(10)	1.134(2)
C(11)-O(11)	1.122(2)
C(12)-O(12)	1.1309(19)
C(13)-O(13)	1.1289(19)
C(14)-O(14)	1.1379(19)

C(10)-Mn-C(14)	93.14(8)
C(10)-Mn-C(12)	90.76(8)
C(14)-Mn-C(12)	176.06(7)
C(10)-Mn-C(11)	93.59(7)
C(14)-Mn-C(11)	89.18(7)
C(12)-Mn-C(11)	90.03(7)
C(10)-Mn-C(13)	92.67(7)
C(14)-Mn-C(13)	90.83(7)
C(12)-Mn-C(13)	89.55(7)
C(11)-Mn-C(13)	173.72(7)
C(10)-Mn-C(9)	178.03(7)
C(14)-Mn-C(9)	85.27(6)
C(12)-Mn-C(9)	90.83(6)
C(11)-Mn-C(9)	85.24(6)
C(13)-Mn-C(9)	88.51(6)
C(1)-C(1A)-C(4A)	119.40(14)
C(1)-C(1A)-C(9)	130.79(14)
C(4A)-C(1A)-C(9)	109.78(12)
C(2)-C(1)-C(1A)	119.30(16)
C(2)-C(1)-H(1)	119.6(10)
C(1A)-C(1)-H(1)	121.1(10)
C(3)-C(2)-C(1)	121.15(17)
C(3)-C(2)-H(2)	121.2(11)
C(1)-C(2)-H(2)	117.4(11)

C(4)-C(3)-C(2)	120.39(16)
C(4)-C(3)-H(3)	122.0(10)
C(2)-C(3)-H(3)	117.6(10)
C(3)-C(4)-C(4A)	119.15(16)
C(3)-C(4)-H(4)	123.6(9)
C(4A)-C(4)-H(4)	117.1(9)
C(4)-C(4A)-C(1A)	120.60(14)
C(4)-C(4A)-C(5A)	130.65(14)
C(1A)-C(4A)-C(5A)	108.63(12)
C(5)-C(5A)-C(8A)	121.15(14)
C(5)-C(5A)-C(4A)	130.70(14)
C(8A)-C(5A)-C(4A)	108.08(12)
C(6)-C(5)-C(5A)	118.72(17)
C(6)-C(5)-H(5)	121.4(9)
C(5A)-C(5)-H(5)	119.7(9)
C(5)-C(6)-C(7)	120.66(18)
C(5)-C(6)-H(6)	119.1(10)
C(7)-C(6)-H(6)	120.1(10)
C(6)-C(7)-C(8)	121.41(18)
C(6)-C(7)-H(7)	119.9(11)
C(8)-C(7)-H(7)	118.6(11)
C(7)-C(8)-C(8A)	119.26(17)
C(7)-C(8)-H(8)	121.3(10)
C(8A)-C(8)-H(8)	119.4(10)
C(8)-C(8A)-C(5A)	118.78(15)
C(8)-C(8A)-C(9)	131.34(14)
C(5A)-C(8A)-C(9)	109.87(12)
C(8A)-C(9)-C(1A)	103.26(11)
C(8A)-C(9)-Mn	111.99(9)
C(1A)-C(9)-Mn	112.38(9)
C(8A)-C(9)-H(9)	112.4(9)

C(1A)-C(9)-H(9)	112.9(10)
Mn-C(9)-H(9)	104.1(9)
O(10)-C(10)-Mn	179.25(19)
O(11)-C(11)-Mn	179.58(16)
O(12)-C(12)-Mn	176.62(15)
O(13)-C(13)-Mn	178.04(14)
O(14)-C(14)-Mn	179.85(18)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{18}\ H_9\ Mn\ O_5$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2} U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn	50(1)	46(1)	47(1)	-6(1)	14(1)	-1(1)
C(1A)	46(1)	37(1)	46(1)	1(1)	6(1)	-4(1)
C(1)	48(1)	54(1)	61(1)	-5(1)	6(1)	-5(1)
C(2)	53(1)	67(1)	66(1)	-2(1)	-9(1)	-8(1)
C(3)	76(1)	59(1)	50(1)	-8(1)	-9(1)	-7(1)
C(4)	71(1)	46(1)	47(1)	-5(1)	7(1)	3(1)
C(4A)	53(1)	35(1)	44(1)	2(1)	7(1)	-2(1)
C(5A)	48(1)	34(1)	50(1)	3(1)	9(1)	-1(1)
C(5)	57(1)	50(1)	67(1)	2(1)	17(1)	4(1)
C(6)	49(1)	57(1)	98(1)	5(1)	17(1)	3(1)
C(7)	50(1)	57(1)	91(1)	11(1)	-10(1)	-2(1)
C(8)	57(1)	50(1)	59(1)	2(1)	-6(1)	-1(1)
C(8A)	47(1)	36(1)	48(1)	4(1)	3(1)	-3(1)
C(9)	50(1)	43(1)	40(1)	-1(1)	8(1)	-4(1)
C(10)	60(1)	56(1)	85(1)	-16(1)	20(1)	-1(1)
C(11)	62(1)	62(1)	57(1)	-6(1)	17(1)	1(1)
C(12)	55(1)	50(1)	61(1)	3(1)	15(1)	4(1)
C(13)	58(1)	41(1)	54(1)	4(1)	12(1)	-1(1)
C(14)	57(1)	64(1)	51(1)	-15(1)	15(1)	-9(1)
O(10)	90(1)	56(1)	153(1)	-27(1)	33(1)	1(1)
O(11)	63(1)	114(1)	92(1)	-3(1)	35(1)	-4(1)
O(12)	87(1)	86(1)	61(1)	14(1)	-1(1)	9(1)
O(13)	60(1)	65(1)	89(1)	16(1)	28(1)	2(1)
O(14)	86(1)	108(1)	50(1)	-13(1)	6(1)	-6(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C_{18} H_9 Mn O_5.

	x	y	z	U(eq)
H(1)	10292(18)	1432(7)	9490(20)	71(5)
H(2)	11210(20)	1796(7)	12480(20)	69(5)
H(3)	9739(19)	2160(7)	14580(30)	75(5)
H(4)	7143(17)	2197(6)	13440(20)	57(5)
H(5)	4483(17)	2192(6)	11660(20)	66(5)
H(6)	2330(20)	2142(7)	9310(20)	72(5)
H(7)	2360(20)	1792(7)	6160(30)	77(6)
H(8)	4512(17)	1482(7)	5270(20)	62(5)
H(9)	7611(16)	1539(6)	6650(20)	52(4)

Table of reaction conditions for the rearrangement 2 → 1

Table of the reaction conditions for the rearrangement 2 → 1.

Entry	Medium	T, °C	t, h	1, %	3, %	ratio 1 : 3
1[a]	THF	66	0.5	80	20	4
2[b]	THF	66	0.5	80	20	4
3[c]	THF	66	0.5	77	23	3.3
4	THF	23	24	23	4	5.8
5	THF	23	48	39	7	5.6
6	THF	23	120	59	12	4.9
7	Ether	35	6	75	10	7.5
8	Ether	35	1.5	38	6	6.3
9	Ether	23	24	14	5	2.8
10	Hexane	69	0.5	60	40	1.5
11[d]	Hexane	23	120	37	17	2.2

12	Nonane	151	0.5	61	39	1.6
13[e]	THF/LiBr	23	22	61	6	10
14[f]	THF/LiCl	23	24	59	7	8.4
15[g]	THF/Bu_4NBr	23	22	63	7	9
16[h]	THF/Bu_4NCl	23	24	59	8	7.4
17[i]	THF/NaBr	23	22	34	8	4.3
18[j]	THF/NaCl	23	24	29	7	4.1
19[k]	THF/$NaBPh_4$	23	24	20	6	3.4
20[l]	THF/LiBr	66	0.5	91	9	10
21[m]	THF/BzBr	66	0.5	73	27	2.7
22[n]	THF/O_2	66	0.5	51	19	2.7
23[o]	THF/CO	66	0.5	64	36	1.8
24[p]	THF/CO	66	1.0	0	33	
25[q]	THF/H_2O	66	0.5	82	8	10

26	2,5-Me_2THF	66	0.5	75	25	3.0
27	2,2,5,5-Me_4THF	66	0.5	72	28	2.6
28	Sealed tube, no solvent	85	6	77	11	7.0

Footnotes: a.) unless otherwise noted, the reactions were carried out at 0.02 M concentrations. The quantities of $Mn_2(CO)_{10}$ matched those of **3**. b.) 0.0026 M concentration c.) 0.00022 M concentration d.) Conversion of **2** to **1** was insufficient for analysis for shorter reaction times e.) LiBr, 0.50 eq. f.) LiCl, 0.58 eq. g.) Bu_4NBr, 0.37 eq. h.) Bu_4NCl, 0.43 eq. i.) NaBr, 0.44 eq. j.) NaCl, 0.60 eq. k.) $NaBPh_4$, 0.39 eq. l.) LiBr, 0.43 eq m.) benzyl bromide, 1.7 eq., additional product: $Mn(CO)_5Br$ (27%), $Mn_2(CO)_{10}$ not found. n.) O_2, 1 atm., additional products: fluorene (11%), fluorenone (8%) o.) CO, 1 atm. p.) CO, 10 atm. q.) H_2O, 0.5 ml, additional product: fluorene (10 %).