Crystal and molecular structures of some phosphane-substituted cymantrenes [(C5H4X)Mn(CO)LL'] (X = H or Cl, L = CO, L' = PPh3 or PCy3, and LL' = Ph2PCH2CH2PPh2)

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UV irradiation of tetrahydrofuran solutions of [CpMn(CO)$_3$] (Cp = π-C$_5$H$_5$ or π-C$_5$H$_4$Cl) in the presence of the phosphanes PPh$_3$ or PCy$_3$ (Cy = cyclohexyl) and Ph$_2$PCH$_2$CH$_2$PPh$_2$ yields the substitution products [CpM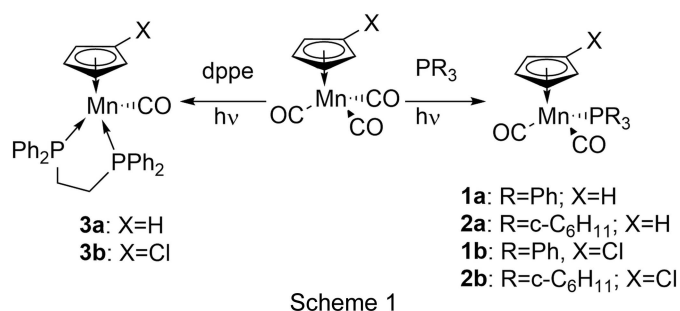n(CO)$_2$PR$_3$] (R = Ph or Cy) and [CpMn(CO)(Ph$_2$PCH$_2$CH$_2$PPh$_2$)], namely, dicarbonyl(η^5-cyclopentadienyl)(triphenylphosphane-κP)manganese(I), [Mn(C$_5$H$_5$)(C$_{18}$H$_{15}$P)(CO)$_2$], 1a, dicarbonyl(η^5-1-chlorocyclopentadienyl)(triphenylphosphane-κP)manganese(I), [Mn(C$_5$H$_4$Cl)(C$_{18}$H$_{15}$P)(CO)$_2$], 1b, dicarbonyl(η^5-cyclopentadienyl)(tricyclohexylphosphane-κP)manganese(I), [Mn(C$_5$H$_5$)(C$_{18}$H$_{33}$P)(CO)$_2$], 2a, dicarbonyl(η^5-1-chlorocyclopentadienyl)(tricyclohexylphosphane-κP)manganese(I), [Mn(C$_5$H$_4$Cl)(C$_{18}$H$_{33}$P)(CO)$_2$], 2b, carbonyl(η^5-cyclopentadienyl)[1,2-bis(diphenylphosphanyl)ethane-$\kappa^2 P,P'$]manganese(I), [Mn(C$_5$H$_5$)(C$_{26}$H$_{24}$P$_2$)(CO)], 3a, and carbonyl(η^5-1-chlorocyclopentadienyl)[1,2-bis(diphenylphosphanyl)ethane-$\kappa^2 P,P'$]manganese(I), [Mn(C$_5$H$_4$Cl)(C$_{26}$H$_{24}$P$_2$)(CO)], 3b, The crystal structure determinations show a very small influence of the chlorine substitution and a moderate influence of the phosphane substitution on the bond lengths. The PR_3 groups avoid being eclipsed with the C—Cl bonds. All the compounds employ weak C—H$\cdots$O interactions for intermolecular association, which are enhanced by C—H$\cdots$Cl contacts in the chlorinated products.

1. Introduction

The substitution of carbon monoxide (CO) by other donor ligands, particularly phosphanes, is one of the most important textbook examples for the reactivity of metal carbonyl complexes (Elschenbroich, 2016; Crabtree, 2005; Jordan, 2007). This is also true for the so-called 'piano-stool' complexes, which contain, besides CO ligands, aromatic π-ligands like benzene or the cyclopentadienyl anion. Many studies have shown that the nature of the π-ligand strongly influences the ease of CO substitution (Veiros, 2000; Le Moigne et al., 1976). But vice versa, the aromatic reactivity depends also on the electronic situation within the metal carbonyl moiety (Fan & Hall, 2001). One of the most studied systems is the 'cymantrene' series CpMn(CO)$_3$ and its substituted derivatives (Caulton, 1981). The substitution of one or two CO ligands by mono- or bidentate phosphanes was studied in the 1960s and it was found that the best way to do this was by UV irradiation (Strohmeier & Barbeau, 1962; Nyholm et al., 1963; Khatami et al., 1972a; Kursanov et al., 1970; Young & Wrighton, 1989). The choice of solvent and the irradiation time were the main determinants for the formation of either mono- or disubstitution products. Later on, studies on the spectroscopic [IR, ESR (electron spin resonance) and NMR] (Rehder & Keçeci, 1985; Ginzburg et al., 1974; Pike et al., 1989) and electro-

chemical properties (Treichel *et al.*, 1975; Connelly & Kitchen, 1977) followed, which showed, as might have been expected, that the introduction of aryl- or alkylphosphanes led to increased electron density at the metal. Further studies were devoted to the reactivity in protonation reactions (Ginzburg *et al.*, 1974), electrophilic hydrogen exchange reactions (Setkina *et al.*, 1973; Khatami *et al.*, 1972b; Antonova & Shapiro, 1991) and deprotonation by butyl lithium (Loim *et al.*, 1988). A survey of the Cambridge Structural Database (CSD, Version 5.42, accessed on 26th August, 2021; Groom *et al.*, 2016) showed no crystal structures for the fragments [(C$_5$H$_4$Cl)Mn-(CO)P] and about 80 entries for the corresponding C$_5$H$_5$-containing fragments. Limitation of the search to the fragment [(C$_5$H$_5$)Mn(CO)$_2$PPh$_2$] gave 10 hits, of which most contained unsymmetrical mono- or dinuclear diphosphanes. Relevant in the context of this study were an early determination of the structure of [(C$_5$H$_5$)Mn(CO)$_2$(PPh$_3$)] (Barbeau *et al.*, 1972) and the crystal structure of [(C$_5$H$_5$)Mn(CO)$_2$PPh$_2$CH$_2$Ph] (CSD refcode GIXRIO; Geicke *et al.*, 1998). No hits were obtained for chelating diphosphanes, except for a derivative of 1,1′-bisdiphenylphosphanylferrocene (EFUHAO; André-Bentabet *et al.*, 2002). We felt it might contribute to a better understanding of this substance class to add some more crystal structure determinations.

Scheme 1

2. Experimental

2.1. Synthesis and crystallization

The syntheses of compounds **1a**, **1b**, **2a** and **3a** have been described previously (Strohmeier & Barbeau, 1962; Khatami *et al.*, 1972a; Strohmeier & Müller, 1967; Nyholm *et al.*, 1963).

2.1.1. General procedure for the synthesis of 1a, 2a and 3a. A solution of [(C$_5$H$_5$)Mn(CO)$_3$] (**I**) and a slight molar excess of the phosphane in tetrahydrofuran (THF, 120 ml) was irradiated for 7 h under argon. The colours of the solutions changed from yellow to red with concomitant gas evolution. After further stirring for 16 h, the solvent was evacuated and the residue dissolved in diethyl ether (Et$_2$O) and filtered through a plug of silica gel. The solvent was evaporated again and the residue dissolved in the minimum amount of petroleum ether. This solution was placed on top of a silica gel chromatography column (alumina in the case of **3a**) and the products were eluted with a petroleum ether/Et$_2$O (9:1 *v/v*) mixture. Evaporation of the eluate yielded the products as yellow powders. Recrystallization from petroleum ether (with

some added Et$_2$O) by slow evaporation in a refrigerator at 5 °C yielded crystals of all three compounds.

Compound **1a** was prepared from **I** (3.00 g, 14.7 mmol) and PPh$_3$ (4.20 g, 16.0 mmol) in a yield of 3.90 g (8.9 ± 0.01 mmol, 61%). 0.57 g of compound **I** (2.8 ± 0.01 mmol, 19%) were recovered. ^{1}H NMR (CDCl$_3$, 400 MHz): δ 7.57–7.20 (*m*, 15H), 4.31 (*s*, 5H). ^{13}C{^{1}H} NMR (CDCl$_3$, 101 MHz): δ 232.8 (*d*, *J* = 26.8 Hz), 138.2 (*d*, *J* = 40.3 Hz), 133.0 (*d*, *J* = 10.6 Hz), 129.6 (*d*, *J* = 2.4 Hz), 128.2 (*d*, *J* = 9.4 Hz), 82.7. ^{31}P{^{1}H} NMR (CDCl$_3$, 162 MHz): δ 93.1.

Compound **2a** was prepared from **I** (0.78 g, 3.8 mmol) and PCy$_3$ (1.12 g, 4.0 mmol) in a yield of 0.11 g (0.24 ± 0.01 mmol, 6%). 0.35 g of compound **I** (1.7 mmol, 45%) were recovered. ^{1}H NMR (CDCl$_3$, 400 MHz): δ 4.48 (*s*, 5H), 2.01–1.11 (*m*, 33H). ^{31}P{^{1}H} NMR (CDCl$_3$, 162 MHz): δ 92.8.

Compound **3a** was prepared from **I** (0.20 g, 1.0 mmol) and 1,2-bis(diphenylphosphanyl)ethane (dppe; 0.44 g, 1.0 mmol) in a yield of 0.15 g (0.27 ± 0.01 mmol, 27%). 0.09 g of compound **I** (0.4 ± 0.01 mmol, 45%) were recovered. ^{1}H NMR (CDCl$_3$, 400 MHz): δ 7.79–7.70 (*m*), 7.44–7.34 (*m*), 7.20–7.11 (*m*), 4.13 (*s*), 2.54–2.41 (*m*), 2.36–2.21 (*m*). ^{31}P{^{1}H} NMR (CDCl$_3$, 162 MHz): δ 118.6.

2.1.2. Synthesis of 1b. Compound **1b** was prepared according to the method reported by Klein-Hessling *et al.* (2021). Recrystallization from petroleum ether (with some added Et$_2$O) by slow evaporation in a refrigerator at 5 °C yielded crystals. ^{1}H NMR (CDCl$_3$, 400 MHz): δ 7.49–7.35 (*m*, 15H), 4.48 (*q*, *J* = 2.0 Hz, 2H), 4.00 (*q*, *J* = 2.3 Hz, 2H). ^{13}C{^{1}H} NMR (CDCl$_3$, 101 MHz): δ 231.8 (*d*, *J* = 23.5 Hz), 137.7 (*d*, *J* = 41.2 Hz), 133.0 (*d*, *J* = 10.5 Hz), 129.8, 128.4 (*d*, *J* = 9.6 Hz), 101.3, 81.5, 81.0. ^{31}P{^{1}H} NMR (CDCl$_3$, 162 MHz): δ 91.8.

2.1.3. Synthesis of 2b. A solution of impure [(C$_5$H$_4$Cl)-Mn(CO)$_3$] (0.50 g, purity *ca* 92%) and PCy$_3$ (0.90 g, 3.2 ± 0.01 mmol) in THF (120 ml) was irradiated for 7 h. After the usual work up (see above), a yellow solid was obtained, consisting of a 7:3 mixture of **2b** and **2a**. Recrystallization from petroleum ether (with some added Et$_2$O) by slow evaporation in a refrigerator at 5 °C yielded crystals. ^{1}H NMR (CDCl$_3$, 270 MHz): δ 4.63 (2H), 4.33 (2H), 2.02–1.07 (33H). ^{31}P{^{1}H} NMR (CDCl$_3$, 162 MHz): δ 91.8. MS (EI, 70 eV): *m/z* = 490.4 (*M*$^+$), 434.4 (*M*$^+$ − 2CO).

2.1.4. Synthesis of 3b. A solution of [(C$_5$H$_4$Cl)Mn(CO)$_3$] (0.35 g, 1.5 ± 0.01 mmol) and dppe (0.62 g, 1.55 ± 0.01 mmol) in THF (120 ml) was irradiated for 7 h. After usual work up, **3b** (0.34 g, 0.6 ± 0.01 mmol, 40%) was isolated as an orange powder. 0.05 g of the starting material (0.25 ± 0.01 mmol, 17%) was recovered. Recrystallization from petroleum ether (with some added Et$_2$O) by slow evaporation in a refrigerator at 5 °C yielded crystals. ^{1}H NMR (CDCl$_3$, 400 MHz): δ 7.82–7.75 (4H), 7.47–7.35 (6H), 7.33–7.22 (6H), 7.19–7.09 (4H), 4.44 (2H), 3.56 (2H), 2.53–2.41 (2H), 2.36–2.22 (2H). ^{13}C{^{1}H} NMR (CD$_2$Cl$_2$, 101 MHz): δ 232.8 (*t*, *J* = 25.2 Hz), 142.9 (*dt*, *J* = 22.4, 11.4 Hz), 139.83–138.89 (*m*), 133.1 (*t*, *J* = 5.4 Hz), 131.4 (*t*, *J* = 4.7 Hz), 129.4, 128.6, 128.1 (*dt*, *J* = 8.7, 4.4 Hz), 97.5, 78.0, 77.9, 77.6, 30.6 (*t*, *J* = 21.2 Hz). ^{31}P{^{1}H} NMR (CDCl$_3$, 162 MHz): δ 117.6. IR (KBr, cm^{-1}): ν (CO) = 1847. MS (EI, 70 eV): *m/z* = 580.3 (*M*$^+$), 552.3 (*M*$^+$ − CO), 398.2 (C$_{26}$H$_{24}$P$_2$), 183.0 (PPh$_2$),

Table 1
Experimental details.

Experiments were carried out with Mo $K\alpha$ radiation using a Bruker D8 Venture (for **1a**, **2b**, **3a** and **3b**) or an Oxford Diffraction KM4 Xcalibur2 (for **1b** and **2a**) diffractometer.

	1a	**1b**	**2a**
Crystal data			
Chemical formula	$[Mn(C_5H_5)(C_{18}H_{15}P)(CO)_2]$	$[Mn(C_5H_4Cl)(C_{18}H_{15}P)(CO)_2]$	$[Mn(C_5H_5)(C_{18}H_{33}P)(CO)_2]$
M_r	438.32	472.76	456.46
Crystal system, space group	Monoclinic, $P2_1/n$	Orthorhombic, $P2_12_12_1$	Monoclinic, $P2_1/n$
Temperature (K)	110	173	173
a, b, c (Å)	7.6736 (4), 15.7356 (8), 33.912 (2)	7.6519 (3), 16.4786 (7), 17.0971 (7)	9.8938 (5), 13.6564 (5), 17.9372 (9)
α, β, γ (°)	90, 95.942 (2), 90	90, 90, 90	90, 105.676 (5), 90
V (Å^3)	4072.9 (4)	2155.82 (15)	2333.42 (19)
Z	8	4	4
μ (mm^{-1})	0.75	0.83	0.65
Crystal size (mm)	$0.05 \times 0.05 \times 0.03$	$0.34 \times 0.14 \times 0.10$	$0.33 \times 0.23 \times 0.14$
Data collection			
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*CrysAlis PRO*; Agilent, 2014)	Multi-scan (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.709, 0.746	0.892, 1	0.990, 1
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	64715, 8968, 7809	14524, 4900, 4297	15861, 5333, 3805
R_{int}	0.048	0.045	0.054
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.641	0.649	0.649
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.090, 1.07	0.038, 0.082, 1.04	0.045, 0.119, 1.03
No. of reflections	8968	4900	5333
No. of parameters	523	271	262
No. of restraints	0	0	1
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.55, −0.65	0.39, −0.29	0.67, −0.47
Absolute structure	–	Flack x determined using 1609 quotients [$(I^+) − (I^-)$]/[$(I^+) + (I^-)$] (Parsons *et al.*, 2013)	–
Absolute structure parameter	–	−0.038 (12)	–

	2b	**3a**	**3b**
Crystal data			
Chemical formula	$[Mn(C_5H_4Cl)(C_{18}H_{33}P)(CO)_2]$	$[Mn(C_5H_5)(C_{26}H_{24}P_2)(CO)]$	$[Mn(C_5H_4Cl)(C_{26}H_{24}P_2)(CO)]$
M_r	490.90	546.43	580.87
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $C2/c$	Triclinic, $P\bar{1}$
Temperature (K)	100	100	100
a, b, c (Å)	9.6649 (3), 13.9301 (4), 17.9790 (6)	29.0323 (7), 8.9592 (2), 26.4794 (7)	8.5739 (5), 11.5697 (8), 14.3909 (9)
α, β, γ (°)	90, 103.835 (1), 90	90, 122.159 (1), 90	90.584 (2), 91.958 (2), 110.490 (2)
V (Å^3)	2350.34 (13)	5830.7 (3)	1336.07 (15)
Z	4	8	2
μ (mm^{-1})	0.76	0.58	0.74
Crystal size (mm)	$0.10 \times 0.08 \times 0.06$	$0.10 \times 0.08 \times 0.07$	$0.08 \times 0.06 \times 0.03$
Data collection			
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.704, 0.745	0.719, 0.746	0.702, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31339, 4809, 4098	70409, 6696, 6042	24803, 5453, 4783
R_{int}	0.039	0.032	0.035
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625	0.650	0.626
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.049, 0.149, 1.06	0.030, 0.081, 1.09	0.027, 0.063, 1.04
No. of reflections	4809	6696	5453
No. of parameters	271	325	334
No. of restraints	1	0	0
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.73, −1.64	0.39, −0.36	0.39, −0.31

Computer programs: *APEX2* (Bruker, 2011), *CrysAlis PRO* (Agilent, 2014), *SAINT* (Bruker, 2011), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXT2018* (Sheldrick, 2015*a*) and *SHELXL2018* (Sheldrick, 2015*b*).
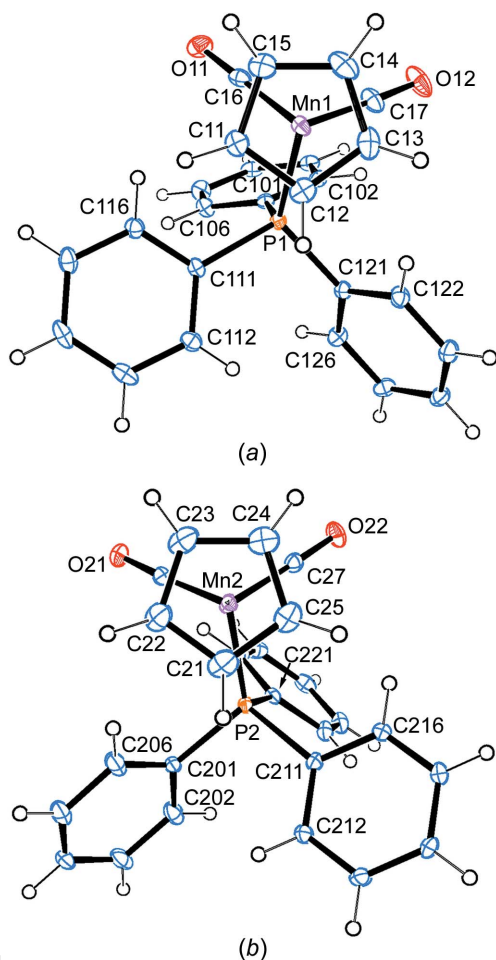
Figure 1
The molecular structures of (*a*) molecule *A* and (*b*) molecule *B* of compound **1a**, with displacement ellipsoids drawn at the 30% probability level.

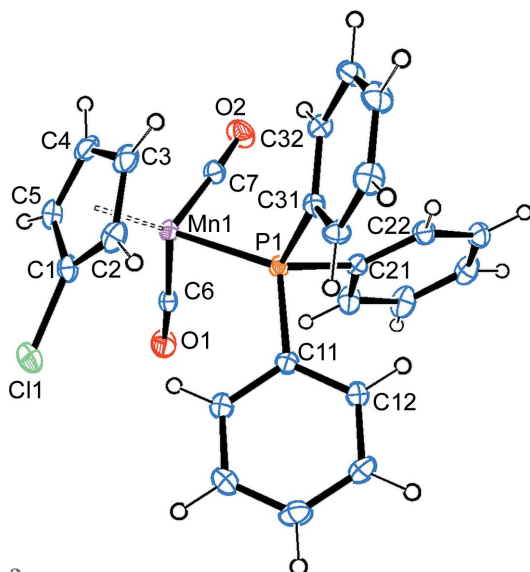108.0 (PPh). HRMS (EI): *m/z* calculated 580.0684, found: 580.0681 (*M*⁺).

Figure 2
The molecular structure (side view) of compound **1b**, with displacement ellipsoids drawn at the 30% probability level.

2.2. Refinement

In the refinements of **2a** and **2b**, a rigid-body restraint was used for the C3—C4 and C2—C3 bonds, respectively, because they had failed the 'Hirshfeld-Test' of *PLATON* (Spek, 2020) significantly. All H atoms were constrained. For compound **3a**, *PLATON* analysis showed 16% solvent-accessible voids. Therefore, the SQUEEZE program (Spek, 2015) was used, which recovered 221 e per unit cell. Crystal data, data collection and structure refinement details are summarized in Table 1.

For the discussion of hydrogen bonds, the standard settings of *Mercury* (Macrae *et al.*, 2020) (H atoms present, $D—H\cdots A$ angle $> 120.0°$, 'all donors', contact distance range 'sum of vdW radii minus 5.00 to sum of vdW radii plus 0.00') were used for all compounds except **1b**, where the 'sum of vdW radii plus 0.10' was used as the upper limit.

3. Results and discussion

3.1. [(C₅H₄*X*)Mn(CO)₂(PPh₃)], *X* = H (1a) and Cl (1b)

Both **1a** and **1b** have been known for some time (Strohmeier & Barbeau, 1962; Khatami *et al.*, 1972*a,b*; Kursanov *et al.*, 1970; Barbeau *et al.*, 1972) and were prepared by irradiation of the corresponding tricarbonyls in the presence of PPh₃. Deprotonation of **1a** with butyl lithium, followed by electronic quenching with C₂Cl₆, yielded **1b** (Klein-Hessling *et al.*, 2021). A crystal structure determination of **1a** had been reported nearly 50 years ago (Barbeau *et al.* 1972). That compound was crystallized from benzene/ethanol in the triclinic space group $P\bar{1}$.

Irradiation of THF solutions of [(C₅H₄*X*)Mn(CO)₃] in the presence of PPh₃ leads to **1a** and **1b** in moderate yields of 40–60% (Scheme 1). Substantial amounts of the starting materials could be recovered. Products were isolated by chromatography and recrystallized from petroleum ether/Et₂O.

3.1.1. Molecular and crystal structure of 1a. The crystals of **1a** obtained from petroleum ether/Et₂O are apparently a different modification than those described in the literature. Our compound crystallized in the monoclinic space group $P2_1/n$ with two independent molecules in the asymmetric unit (Fig. 1).

The major difference between the two molecules is in the relative orientation of the Mn(CO)₂P tripod and the projection of the cyclopentadienyl ring. While in molecule *A* both Mn→P and one Mn→CO vector nearly eclipse C—H bonds of the cyclopentadienyl ring, in molecule *B* this is the case for the Mn→P vector only. In addition, the Mn2—P2 bond [2.2421 (7) Å] is significantly longer (>20σ) than the Mn1—P1 bond [2.2259 (6) Å]. All other bond lengths are identical in the two molecules (Table 2).

There are five intermolecular C—H⋯O hydrogen bonds (Table S1 in the supporting information). Three of them involve arene C—H bonds, and carbonyl atom O22 accepts two of them (Fig. S1).

3.1.2. Molecular structure of 1b. Compound **1b** crystallizes in the acentric orthorhombic space group $P2_12_12_1$ with one molecule in the asymmetric unit (Fig. 2). Examination by the

Table 2
Important bond parameters of **1–3** in comparison with two related literature compounds.

Ct is the centroid of the cyclopentadienyl ring, $(C-C)_{av}$ is the average C—C bond length within the cyclopentadienyl ring and C_x—Ct—Mn—P is the smallest torsion angle involving a cyclopentadienyl C—H (**1a**, **2a** and **3a**) or C—Cl bond.

Distance/angle	1a mol. A/ mol. B	1b	2a	2b	3a	3b	GIXRIO	EFUHAO
Mn—Ct	1.777 (1)/1.778 (1)	1.786 (2)	1.781 (1)	1.786 (1)	1.761 (2)	1.768 (1)	1.773 (2)	1.769 (9)
Mn—P	2.2256 (8)/2.2423 (8)	2.2403 (10)	2.2661 (7)	2.2743 (9)	2.1968 (4), 2.1849 (4)	2.1961 (5), 2.2024 (5)	2.2198 (2)	2.244 (3), 2.241 (3)
Mn—CO	1.769 (2), 1.776 (2)/ 1.777 (2), 1.767 (2)	1.772 (4), 1.770 (3)	1.763 (2), 1.761 (2)	1.774 (3), 1.773 (3)	1.756 (5)	1.755 (2)	1.755 (5)	1.769 (9)
C—O	1.165 (3), 1.162 (3)/ 1.162 (3), 1.160 (3)	1.155 (5), 1.164 (4)	1.162 (3), 1.174 (4)	1.161 (4), 1.162 (4)	1.174 (6)	1.172 (2)	1.161 (7), 1.165 (6)	1.15 (1)
C—Cl	–	1.730 (4)	–	1.674 (4)	–	1.737 (2)	–	–
$(C-C)_{av}$	1.416 (3)/1.415 (4)	1.408 (5)	1.408 (4)	1.411 (6)	1.422 (5)	1.416 (2)	1.395 (7)	1.41 (2)
C_{Cl}—Ct—Mn—P	–	77.6	–	78.0	–	36.3, 156.0	–	–
C_H—Ct—Mn—P	13.0/8.1	20.5	12.3	7.2	14.1, 13.4	36.0, 12.1	10.2	4.4, 13.6

program *PLATON* (Spek, 2020) showed no extra crystallographic symmetry and no sign of racemic twinning. The only 'molecular' origin of chirality resides in the PPh$_3$ 'propeller'.

The Mn→P vector is nearly perpendicular to the C—Cl bond (torsion angle C1—Ct—Mn—P1 is 77.6°). The individual bond lengths are nearly identical to those in **1a**; the largest deviation is found for the C—C bonds of the cyclopentadienyl ring, which are slightly (1.5σ) shorter in **1b**. The most important bond parameters can be found in Table 2.

There is only one intramolecular C—H···Cl hydrogen bond with a length shorter than the sum of the van der Waals radii (H16···Cl1). Additionally, there is one weak intramolecular and three intermolecular C—H···O hydrogen bonds, and one intermolecular C—H···Cl hydrogen bond (Fig. S2 and Table S1 in the supporting information). The Cl atoms always

bridge two different H atoms of the same symmetry-related arene ring along the *a* screw axis. Apparently, this interaction enforces the orientation of this particular arene ring and generates the chirality.

3.2. [(C$_5$H$_4$X)Mn(CO)$_2$(PCy$_3$)], X = H (2a) and Cl (2b)

The tricyclohexylphosphane compound **2a** was first described in 1967 (Strohmeier & Müller, 1967) as part of a study on the π-acceptor strength of phosphane ligands. It was then characterized by IR spectroscopy and elemental analysis. Later on it was shown that its reactivity in hydrogen isotope exchange reactions was more than 15 times greater in comparison to the PPh$_3$ compound **1a** (Setkina *et al.*, 1973). Further spectroscopic characterizations (^{13}C and ^{31}P NMR) and protonation studies followed soon afterwards (Ginzburg
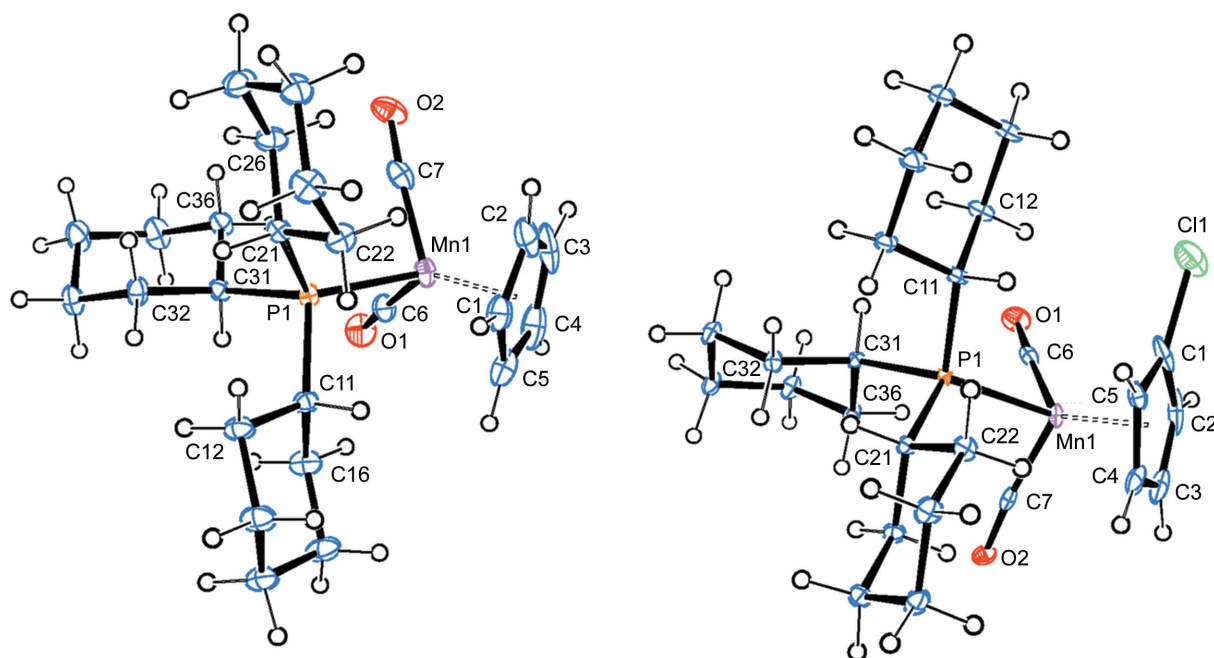

Figure 3
The molecular structures (side view) of compounds **2a** (left) and **2b** (right), with displacement ellipsoids drawn at the 30% probability level.

et al., 1974). The chlorocyclopentadienyl complex **2b** has not been reported before.

We prepared both compounds according to Scheme 1 *via* irradiation of the corresponding tricarbonyl complexes in the presence of PCy$_3$ (tricyclohexylphosphane) in very low yield. Despite long irradiation times, large amounts of the starting material could be recovered. In contrast to **1a**, it was not possible to lithiate **2a** with *n*-BuLi or *t*-BuLi and chlorinate the presumed intermediate lithium compound with C$_2$Cl$_6$ to give **2b**. It was possible, however, to obtain crystals of both compounds suitable for X-ray diffraction.

3.2.1. Molecular structure of 2a. Compound **2a** crystallizes in the monoclinic space group $P2_1/n$, with one molecule in the asymmetric unit (Fig. 3). The Mn→P vector nearly eclipses a C—H bond of the cyclopentadienyl ring. While the Mn—P bond [2.2661 (7) Å] is significantly longer (50σ) than the average Mn—P bond in **1a**, the Mn—CO bonds are slightly shorter (3–5σ) (Table 2). The distance from manganese to the cyclopentadienyl centroid is slightly longer (3σ) in **2a** compared to **1a**.

There is one intramolecular and two intermolecular C—H···O hydrogen bonds involving exclusively methylene H atoms of the PCy$_3$ ligand and carbonyl atom O1. A packing diagram shows that these interactions mainly (although not exclusively) join the individual molecules in the *c* direction (Fig. S3 and Table S1 in the supporting information).

3.2.2. Molecular structure of 2b. Compound **2b** crystallizes in the monoclinic space group $P2_1/c$, with one molecule in the asymmetric unit (Fig. 3). The Mn→P vector is nearly perpendicular to the C—Cl bond (torsion angle C1—Ct—Mn1—P1 is 78°), with the Mn—P bond [2.2743 (9) Å] being significantly longer (8σ) than in **2a**. The Mn—CO bonds are slightly longer (3σ) than in **2a** and have the same lengths as in **1b**. This is also true for the distance of the Mn atom from the centroid of the cyclopentadienyl ring. More bond parameters can be found in Table 2.

There are intramolecular C—H···X interactions involving two methylene H atoms of the PCy$_3$ ligand and either the Cl atom or one carbonyl O atom. Additionally, an intermolecular C—H···Cl hydrogen bond joins glide-plane-related molecules along the *b* axis (Fig. S4 and Table S1 in the supporting information).

3.3. [(C$_5$H$_4$X)Mn(CO)(dppe)], with X = H (3a) and Cl (3b)

The monocarbonyl chelate complex **3a** was first prepared by the photochemical reaction of cymantrene with bis(diphenylphosphanyl)ethane (dppe) in benzene (*ca* 85% yield after 50 h irradiation), while the same reaction in cyclohexane produced the dppe-bridged dinuclear complex {[(C$_5$H$_5$)Mn(CO)$_2$]$_2$[μ-dppe]} (Nyholm *et al.*, 1963). Among several studies devoted to spectroscopic characterization and general reactivity, it was found that **3a** had a ninefold decreased kinetic acidity when compared to cymantrene (Antonova & Shapiro, 1991). Compound **3b** has not been reported previously.

Irradiation of THF solutions of the corresponding tricarbonyl complexes in the presence of dppe for 7 h yields **3a** and **3b** in modest yields (30–40%), again with substantial recovery of the starting material. Some weak signals in the NMR spectra showed small amounts of other products, most likely dinuclear ones. However, the influence of prolonged reaction times on product yields and distribution was not examined. In contrast to the reactivity of **1b**, it was not possible to deprotonate **3b** [either by lithium diisopropylamide (LDA), lithium tetramethylpiperidide (LiTMP) or *t*-BuLi] and introduce more chlorine substituents *via* addition of C$_2$Cl$_6$. However, again it was possible to obtain crystals suitable for X-ray diffraction for both compounds.

3.3.1. Molecular structure of 3a. Compound **3a** crystallizes in the monoclinic space group $C2/c$, with one molecule in the asymmetric unit. Fig. 4 shows a top view of the molecular structure. Both Mn→P vectors nearly eclipse two C—H bonds in mutual 1- and 3-positions of the cyclopentadienyl ring, while the Mn→CO vector bisects a C—C bond. The Mn—P [2.1968 (4) and 2.1849 (4) Å] and Mn—CO [1.7549 (15) Å] bonds, as well as the distance from manganese to the cyclopentadienyl centroid [1.761 (2) Å], are shorter than for all the above-mentioned compounds. At the same time, the C—C
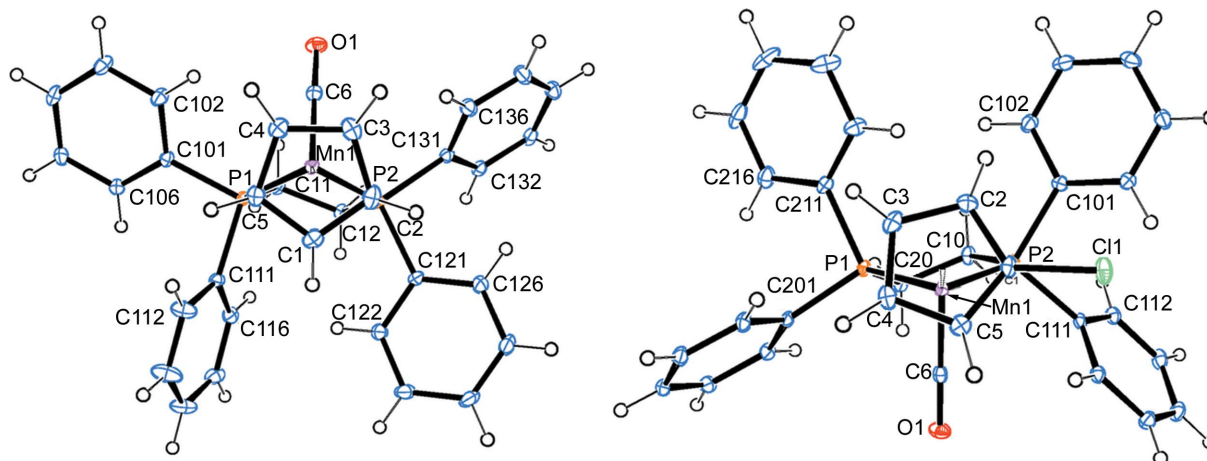

Figure 4
The molecular structures (top views) of compounds **3a** (left) and **3b** (right), with displacement ellipsoids drawn at the 30% probability level.

bonds of the cyclopentadienyl rings are longer than in the other compounds (Table 2).

There are two intermolecular hydrogen bonds involving the carbonyl O atom and one methylene H atom of the PCy_3 ligand or one C—H group of the cyclopentadienyl ring. The packing diagram shows that these interactions connect the individual molecules in the *a* direction (Fig. S5 and Table S1 in the supporting information).

3.3.2. Molecular structure of 3b. Compound **3b** crystallizes in the triclinic space group $P\bar{1}$, with one molecule in the asymmetric unit (Fig. 4). The Mn→P2 vector bisects the C—C bond next to the chlorine substituent, while the Mn→P1 and Mn→CO vectors nearly eclipse two C—H bonds in the 2- and 4-positions. The Mn—P bond lengths [2.1961 (5) and 2.2024 (5) Å] are significantly different from each other (by 12σ) and slightly longer than in **3a**. The same holds for the relative distances between manganese and the cyclopentadienyl centroids, while the Mn—CO bonds are virtually identical (Table 2). It is worth noting the near perpendicular orientation of one arene ring (C201–C206) relative to the cyclopentadienyl ring (interplanar angle 86.0°). This leads to a rather close approach of arene H atom H206 to cyclopentadienyl atom H4 (2.375 Å).

There is one intermolecular C—H⋯Cl hydrogen bond involving an arene H atom, which joins the individual molecules in the *b* direction. The carbonyl O atom joins two molecules in the *a* direction, employing one arene H atom and one cyclopentadienyl H atom each (Fig. S6 and Table S1 in the supporting information).

4. Comparison of the structures and conclusion

The introduction of a chlorine substituent in the cyclopentadienyl ring leads to a slight increase in the Mn—Ct and Mn—P distances for all the title phosphanes, while both the Mn—CO and the C—O bonds are only affected in the PCy_3 system, where a substantial elongation occurs. When comparing the two triads with different phosphanes, the Mn—Ct (Ct describes the centroid of the cyclopentadienyl ring) and Mn—P distances show a slight increase in the order $3\rightarrow1\rightarrow2$. The C—O bonds follow the trend $1 \simeq 2 < 3$ and the C—Cl bonds follow the trend $2b < 1b \simeq 3b$. The average C—C bond lengths are the same within 2σ for all six compounds. Comparison with the PPh_2CH_2Ph compound GIXRIO and the ferrocenylbisphosphane chelate compound EFUHAO shows more similarities with the PPh_3 complexes **1** than with the dppe chelates **3**. The tendency of the Mn—P bonds to eclipse one cyclopentadienyl C—H bond is obvious in all the compounds. In all the chloro compounds, the Mn—P bonds avoid being eclipsed with the C—Cl bond of the cyclopentadienyl ring.

Apparently, the introduction of one chlorine substituent has only a small influence on the bond lengths, despite the relatively large effect on the spectroscopic data. Steric hindrance within the phosphanes seems to be of greater importance for the bond parameters than the differences in electronic effects. However, the presence of chlorine in the cyclopentadienyl ring leads to additional lattice stabilization *via* the formation of C—H⋯Cl hydrogen bonds.

References

Agilent (2014). *CrysAlis PRO*. Agilent Technologies Ltd, Yarnton, Oxfordshire, England.

André-Bentabet, E., Broussier, R., Amardeil, R., Hierso, J.-C., Richard, P., Fasseur, D., Gautheron, B. & Meunier, P. (2002). *J. Chem. Soc. Dalton Trans.* pp. 2322–2327.

Antonova, M. V. & Shapiro, I. O. (1991). *Metalloorg. Khim.* **4**, 674–675.

Barbeau, C., Sorrento Dichmann, K. & Ricard, L. (1972). *Can. J. Chem.* **31**, 3027–3031.

Bruker (2011). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Caulton, C. G. (1981). *Coord. Chem. Rev.* **38**, 1–43.

Connelly, N. G. & Kitchen, M. D. (1977). *J. Chem. Soc. Dalton Trans.* pp. 931–937.

Crabtree, R. H. (2005). *The Organometallic Chemistry of the Transition Metals*, 4th ed., edited by R. H. Crabtree, pp. 87–124. Chichester: Wiley.

Elschenbroich, C. (2016). *Organometallics*, 3rd ed, ch. 14.4. Chichester: John Wiley & Sons.

Fan, H.-J. & Hall, M. B. (2001). *Organometallics*, **20**, 5724–5730.

Geicke, J., Lorenz, I. P. & Polborn, K. (1998). *Inorg. Chim. Acta*, **272**, 101–108.

Ginzburg, A. G., Fedorov, L. A., Petrovskii, P. V., Fedin, E. I., Setkina, V. N. & Kursanov, D. N. (1974). *J. Organomet. Chem.* **73**, 77–84.

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.

Jordan, R. B. (2007). *Reaction Mechanisms of Inorganic and Organometallic Systems*, ch. 5.1. Oxford University Press.

Khatami, A. I., Ginzburg, A. G., Nefedova, M. N., Setkina, V. N. & Kursanov, D. N. (1972a). *Zh. Obsch. Khim.* **42**, 2665–2667.

Khatami, A. I., Nefedova, M. N., Setkina, V. N. & Kursanov, D. N. (1972b). *Dokl. Akad. Nauk SSSR*, **203**, 1094–1096.

Klein-Hessling, C., Blockhaus, T. & Sünkel, K. (2021). *J. Organomet. Chem.* **943**, 121833.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Kursanov, D. N., Setkina, V. N., Ginzburg, A. G., Nefedova, M. N. & Khatami, A. I. (1970). *Izv. Akad. Nauk. SSSR*, p. 2412.

Le Moigne, F., Dabard, R. & Le Plouzennec, M. (1976). *J. Organomet. Chem.* **122**, 365–376.

Loim, N. M., Barsegova, M. N. & Ginzburg, A. G. (1988). *Metalloorg. Khim.* **1**, 889–892.

Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.

Nyholm, R. S., Sandhu, S. S. & Stiddard, M. H. B. (1963). *J. Chem. Soc.* pp. 5916–5919.

Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.

Pike, R. D., Rieger, A. L. & Rieger, P. H. (1989). *J. Chem. Soc. Faraday Trans. 1*, **85**, 3913.

Rehder, D. & Keçeci, A. (1985). *Inorg. Chim. Acta*, **103**, 173–177.

Setkina, V. N., Baranetskaya, N. K., Ginzburg, A. G., Zdanovich, V. I., Nefedova, M. N. & Kursanov, D. N. (1973). *J. Organomet. Chem.* **61**, 287–300.

Sheldrick, G. M. (2015a). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015b). *Acta Cryst.* C**71**, 3–8.

Spek, A. L. (2015). *Acta Cryst.* C**71**, 9–18.

Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

Strohmeier, W. & Barbeau, C. (1962). *Z. Naturforsch. B*, **17**, 818–819.

Strohmeier, W. & Müller, F.-J. (1967). *Chem. Ber.* **100**, 2812–2821.

Treichel, P. M., Wagner, K. P. & Mueh, H. J. (1975). *J. Organomet. Chem.* **86**, C13–C16.

Veiros, L. F. (2000). *Organometallics*, **19**, 3127–3136.

Young, K. M. & Wrighton, M. S. (1989). *Organometallics*, **8**, 1063–1066.

Crystal and molecular structures of some phosphane-substituted cymantrenes [(C₅H₄*X*)Mn(CO)*LL*′] (*X* = H or Cl, *L* = CO, *L*′ = PPh₃ or PCy₃, and *LL*′ = Ph₂PCH₂CH₂PPh₂)

Karlheinz Sünkel and Christian Klein-Hessling

Computing details

Data collection: *APEX2* (Bruker, 2011) for compd1a, compd2b, compd3a, compd3b; *CrysAlis PRO* (Agilent, 2014) for compd1b, compd2a. Cell refinement: *APEX2* (Bruker, 2011) for compd1a, compd2b, compd3a, compd3b; *CrysAlis PRO* (Agilent, 2014) for compd1b, compd2a. Data reduction: *SAINT* (Bruker, 2011) for compd1a, compd2b, compd3a, compd3b; *CrysAlis PRO* (Agilent, 2014) for compd1b, compd2a. Program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a) for compd1a, compd1b, compd2a, compd2b, compd3b; SHELXT2018 (Sheldrick, 2015a) for compd3a. For all structures, program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b).

Dicarbonyl(η⁵-cyclopentadienyl)(triphenylphosphane-κ*P*)manganese(I) (compd1a)

Crystal data

[Mn(C₅H₅)(C₁₈H₁₅P)(CO)₂]	$F(000) = 1808$
$M_r = 438.32$	$D_x = 1.430$ Mg m⁻³
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.6736$ (4) Å	Cell parameters from 9770 reflections
$b = 15.7356$ (8) Å	$\theta = 2.7–27.1°$
$c = 33.912$ (2) Å	$\mu = 0.75$ mm⁻¹
$\beta = 95.942$ (2)°	$T = 110$ K
$V = 4072.9$ (4) Å³	Block, yellow
$Z = 8$	$0.05 \times 0.05 \times 0.03$ mm

Data collection

Bruker D8 Venture diffractometer	64715 measured reflections
	8968 independent reflections
Radiation source: rotating anode generator	7809 reflections with $I > 2\sigma(I)$
Detector resolution: 7.391 pixels mm⁻¹	$R_{int} = 0.048$
mix of ω and phi scans	$\theta_{max} = 27.1°$, $\theta_{min} = 2.2°$
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)	$h = -9 \rightarrow 9$
	$k = -20 \rightarrow 20$
$T_{min} = 0.709$, $T_{max} = 0.746$	$l = -43 \rightarrow 43$

Refinement

Refinement on F^2	8968 reflections
Least-squares matrix: full	523 parameters
$R[F^2 > 2\sigma(F^2)] = 0.038$	0 restraints
$wR(F^2) = 0.090$	Primary atom site location: dual
$S = 1.07$	

Hydrogen site location: inferred from neighbouring sites	$w = 1/[\sigma^2(F_o^2) + (0.0276P)^2 + 5.0438P]$ where $P = (F_o^2 + 2F_c^2)/3$
H-atom parameters constrained	$(\Delta/\sigma)_{max} = 0.001$
	$\Delta\rho_{max} = 0.55$ e Å^{-3}
	$\Delta\rho_{min} = -0.65$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Mn1	0.85454 (4)	0.19579 (2)	0.67910 (2)	0.01828 (8)
P1	0.73804 (6)	0.28831 (3)	0.71853 (2)	0.01491 (11)
C11	1.1174 (3)	0.17804 (14)	0.70677 (7)	0.0235 (5)
H11	1.193292	0.222944	0.716205	0.028*
C12	1.0005 (3)	0.13330 (14)	0.72884 (7)	0.0254 (5)
H12	0.984055	0.143119	0.755842	0.030*
C13	0.9123 (3)	0.07157 (14)	0.70398 (8)	0.0303 (5)
H13	0.826935	0.032542	0.711328	0.036*
C14	0.9740 (3)	0.07820 (15)	0.66602 (8)	0.0330 (6)
H14	0.936847	0.044647	0.643412	0.040*
C15	1.1002 (3)	0.14347 (15)	0.66793 (7)	0.0280 (5)
H15	1.163359	0.161356	0.646739	0.034*
C16	0.8850 (3)	0.27855 (14)	0.64521 (6)	0.0220 (4)
C17	0.6483 (3)	0.16736 (15)	0.65394 (7)	0.0288 (5)
O11	0.9126 (2)	0.33197 (11)	0.62291 (5)	0.0318 (4)
O12	0.5185 (2)	0.14436 (12)	0.63652 (6)	0.0438 (5)
C101	0.6000 (3)	0.37102 (13)	0.69258 (6)	0.0164 (4)
C102	0.4413 (3)	0.34694 (13)	0.67145 (6)	0.0198 (4)
H102	0.405493	0.289162	0.671610	0.024*
C103	0.3355 (3)	0.40626 (15)	0.65028 (6)	0.0227 (4)
H103	0.228223	0.388841	0.636103	0.027*
C104	0.3858 (3)	0.49091 (14)	0.64972 (6)	0.0240 (5)
H104	0.313675	0.531441	0.635078	0.029*
C105	0.5416 (3)	0.51582 (14)	0.67062 (7)	0.0273 (5)
H105	0.576460	0.573735	0.670396	0.033*
C106	0.6480 (3)	0.45647 (13)	0.69203 (6)	0.0224 (4)
H106	0.754444	0.474430	0.706413	0.027*
C111	0.8995 (3)	0.35271 (12)	0.74917 (6)	0.0172 (4)
C112	0.8897 (3)	0.36919 (14)	0.78919 (6)	0.0231 (4)
H112	0.802080	0.342276	0.802631	0.028*
C113	1.0077 (3)	0.42495 (15)	0.80964 (7)	0.0295 (5)
H113	0.999684	0.435950	0.836938	0.035*
C114	1.1363 (3)	0.46444 (14)	0.79053 (7)	0.0300 (5)
H114	1.213755	0.503974	0.804361	0.036*

C115	1.1515 (3)	0.44600 (14)	0.75114 (7)	0.0255 (5)
H115	1.241859	0.471526	0.738076	0.031*
C116	1.0348 (3)	0.39030 (13)	0.73074 (6)	0.0208 (4)
H116	1.046990	0.377456	0.703793	0.025*
C121	0.5917 (3)	0.24949 (13)	0.75399 (6)	0.0169 (4)
C122	0.5862 (3)	0.16338 (14)	0.76309 (7)	0.0222 (4)
H122	0.656269	0.124327	0.750313	0.027*
C123	0.4789 (3)	0.13418 (14)	0.79078 (7)	0.0263 (5)
H123	0.477895	0.075423	0.797185	0.032*
C124	0.3739 (3)	0.18983 (15)	0.80905 (7)	0.0242 (5)
H124	0.299947	0.169375	0.827753	0.029*
C125	0.3767 (3)	0.27557 (15)	0.80001 (7)	0.0251 (5)
H125	0.304373	0.314099	0.812470	0.030*
C126	0.4854 (3)	0.30524 (14)	0.77272 (6)	0.0219 (4)
H126	0.487297	0.364193	0.766742	0.026*
Mn2	0.58566 (4)	0.16120 (2)	0.42672 (2)	0.02007 (8)
P2	0.75532 (7)	0.24724 (3)	0.46702 (2)	0.01895 (12)
C21	0.4526 (4)	0.12059 (16)	0.47594 (8)	0.0360 (6)
H21	0.487507	0.136169	0.502652	0.043*
C22	0.5107 (4)	0.04810 (15)	0.45630 (8)	0.0372 (6)
H22	0.590921	0.006526	0.467502	0.045*
C23	0.4279 (4)	0.04866 (16)	0.41692 (8)	0.0356 (6)
H23	0.442709	0.007495	0.397052	0.043*
C24	0.3195 (3)	0.12124 (17)	0.41250 (8)	0.0347 (6)
H24	0.248934	0.137633	0.389071	0.042*
C25	0.3345 (3)	0.16552 (16)	0.44923 (8)	0.0330 (6)
H25	0.275176	0.216472	0.454726	0.040*
C26	0.7653 (3)	0.11595 (13)	0.40507 (6)	0.0238 (5)
C27	0.5568 (3)	0.24139 (13)	0.39010 (6)	0.0204 (4)
O21	0.8763 (2)	0.08380 (11)	0.38960 (5)	0.0326 (4)
O22	0.5301 (2)	0.29233 (10)	0.36554 (5)	0.0297 (4)
C201	0.9218 (3)	0.19896 (15)	0.50301 (6)	0.0246 (5)
C202	1.0608 (3)	0.24533 (17)	0.52160 (7)	0.0294 (5)
H202	1.075712	0.303089	0.514518	0.035*
C203	1.1787 (3)	0.20805 (18)	0.55054 (7)	0.0342 (6)
H203	1.273940	0.240137	0.562932	0.041*
C204	1.1566 (4)	0.12431 (18)	0.56117 (7)	0.0406 (7)
H204	1.236939	0.098886	0.580891	0.049*
C205	1.0182 (5)	0.07731 (18)	0.54327 (9)	0.0538 (9)
H205	1.002150	0.020021	0.550959	0.065*
C206	0.9022 (4)	0.11449 (17)	0.51386 (8)	0.0462 (8)
H206	0.808821	0.081763	0.501093	0.055*
C211	0.6293 (3)	0.31214 (13)	0.49899 (6)	0.0188 (4)
C212	0.6646 (3)	0.31426 (14)	0.54006 (6)	0.0228 (4)
H212	0.758496	0.281595	0.552688	0.027*
C213	0.5629 (3)	0.36407 (15)	0.56272 (7)	0.0268 (5)
H213	0.588103	0.365541	0.590740	0.032*
C214	0.4252 (3)	0.41147 (15)	0.54459 (7)	0.0258 (5)

H214	0.355729	0.445217	0.560126	0.031*
C215	0.3890 (3)	0.40957 (14)	0.50369 (7)	0.0247 (5)
H215	0.295116	0.442376	0.491176	0.030*
C216	0.4893 (3)	0.36003 (14)	0.48109 (6)	0.0229 (4)
H216	0.462911	0.358491	0.453105	0.027*
C221	0.8851 (3)	0.32809 (14)	0.44380 (6)	0.0202 (4)
C222	0.8888 (3)	0.41354 (14)	0.45507 (7)	0.0253 (5)
H222	0.820547	0.431825	0.475315	0.030*
C223	0.9907 (3)	0.47224 (15)	0.43713 (7)	0.0293 (5)
H223	0.989093	0.530341	0.444700	0.035*
C224	1.0944 (3)	0.44648 (16)	0.40834 (7)	0.0303 (5)
H224	1.165649	0.486403	0.396437	0.036*
C225	1.0933 (3)	0.36201 (17)	0.39705 (7)	0.0312 (5)
H225	1.164519	0.343855	0.377343	0.037*
C226	0.9889 (3)	0.30359 (16)	0.41429 (7)	0.0275 (5)
H226	0.988091	0.245992	0.405888	0.033*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.01353 (15)	0.01902 (16)	0.02168 (17)	0.00274 (12)	−0.00109 (12)	−0.00469 (12)
P1	0.0134 (2)	0.0143 (2)	0.0166 (2)	0.00031 (18)	−0.00035 (19)	−0.00050 (19)
C11	0.0153 (10)	0.0248 (11)	0.0292 (12)	0.0054 (8)	−0.0031 (8)	0.0008 (9)
C12	0.0218 (11)	0.0263 (11)	0.0279 (12)	0.0085 (9)	0.0017 (9)	0.0048 (9)
C13	0.0209 (11)	0.0180 (11)	0.0516 (16)	0.0038 (9)	0.0024 (10)	0.0012 (10)
C14	0.0282 (12)	0.0281 (12)	0.0412 (14)	0.0123 (10)	−0.0027 (10)	−0.0136 (11)
C15	0.0192 (11)	0.0328 (12)	0.0320 (12)	0.0110 (9)	0.0031 (9)	−0.0015 (10)
C16	0.0157 (10)	0.0310 (12)	0.0184 (10)	0.0042 (9)	−0.0021 (8)	−0.0056 (9)
C17	0.0218 (11)	0.0257 (11)	0.0382 (13)	0.0049 (9)	−0.0008 (10)	−0.0123 (10)
O11	0.0287 (9)	0.0444 (10)	0.0215 (8)	0.0022 (8)	−0.0014 (7)	0.0065 (7)
O12	0.0235 (9)	0.0434 (11)	0.0614 (13)	0.0012 (8)	−0.0107 (9)	−0.0247 (10)
C101	0.0163 (9)	0.0184 (9)	0.0148 (9)	0.0039 (8)	0.0032 (7)	0.0002 (7)
C102	0.0191 (10)	0.0207 (10)	0.0198 (10)	0.0003 (8)	0.0032 (8)	−0.0006 (8)
C103	0.0165 (10)	0.0340 (12)	0.0173 (10)	0.0045 (9)	0.0004 (8)	0.0008 (9)
C104	0.0270 (11)	0.0275 (11)	0.0173 (10)	0.0118 (9)	0.0008 (9)	0.0034 (8)
C105	0.0333 (12)	0.0183 (10)	0.0298 (12)	0.0042 (9)	0.0014 (10)	0.0037 (9)
C106	0.0218 (11)	0.0201 (10)	0.0242 (11)	0.0018 (8)	−0.0031 (9)	−0.0001 (8)
C111	0.0166 (9)	0.0145 (9)	0.0194 (10)	0.0011 (8)	−0.0029 (8)	0.0002 (7)
C112	0.0219 (11)	0.0248 (11)	0.0217 (11)	0.0018 (9)	−0.0021 (8)	0.0001 (9)
C113	0.0328 (13)	0.0312 (12)	0.0226 (11)	0.0040 (10)	−0.0069 (10)	−0.0078 (9)
C114	0.0286 (12)	0.0210 (11)	0.0374 (13)	−0.0028 (9)	−0.0116 (10)	−0.0052 (10)
C115	0.0214 (11)	0.0197 (10)	0.0337 (13)	−0.0020 (9)	−0.0050 (9)	0.0051 (9)
C116	0.0190 (10)	0.0221 (10)	0.0204 (10)	0.0001 (8)	−0.0018 (8)	0.0011 (8)
C121	0.0139 (9)	0.0185 (10)	0.0178 (10)	−0.0001 (8)	−0.0007 (7)	0.0005 (8)
C122	0.0217 (10)	0.0191 (10)	0.0260 (11)	0.0006 (8)	0.0041 (9)	−0.0031 (8)
C123	0.0301 (12)	0.0195 (10)	0.0295 (12)	−0.0037 (9)	0.0044 (10)	0.0033 (9)
C124	0.0212 (11)	0.0302 (12)	0.0216 (11)	−0.0030 (9)	0.0042 (8)	0.0031 (9)
C125	0.0234 (11)	0.0299 (12)	0.0230 (11)	0.0045 (9)	0.0065 (9)	0.0011 (9)

C126	0.0219 (10)	0.0196 (10)	0.0242 (11)	0.0034 (8)	0.0028 (8)	0.0029 (8)
Mn2	0.03021 (18)	0.01543 (15)	0.01517 (16)	0.00275 (13)	0.00515 (13)	0.00225 (12)
P2	0.0255 (3)	0.0184 (3)	0.0130 (2)	0.0089 (2)	0.0018 (2)	0.00046 (19)
C21	0.0540 (16)	0.0306 (13)	0.0264 (12)	−0.0077 (12)	0.0185 (12)	0.0038 (10)
C22	0.0623 (18)	0.0208 (11)	0.0304 (13)	−0.0008 (12)	0.0145 (12)	0.0073 (10)
C23	0.0548 (17)	0.0238 (12)	0.0305 (13)	−0.0116 (11)	0.0153 (12)	−0.0003 (10)
C24	0.0348 (13)	0.0363 (14)	0.0342 (14)	−0.0127 (11)	0.0089 (11)	0.0008 (11)
C25	0.0356 (13)	0.0291 (12)	0.0374 (14)	−0.0039 (11)	0.0193 (11)	0.0023 (10)
C26	0.0350 (12)	0.0180 (10)	0.0174 (10)	0.0053 (9)	−0.0023 (9)	0.0016 (8)
C27	0.0183 (10)	0.0216 (10)	0.0216 (10)	0.0014 (8)	0.0042 (8)	−0.0022 (8)
O21	0.0371 (10)	0.0298 (9)	0.0310 (9)	0.0148 (8)	0.0035 (7)	−0.0055 (7)
O22	0.0328 (9)	0.0274 (8)	0.0288 (9)	0.0058 (7)	0.0022 (7)	0.0140 (7)
C201	0.0311 (12)	0.0291 (11)	0.0132 (10)	0.0157 (10)	0.0009 (8)	−0.0020 (8)
C202	0.0236 (11)	0.0393 (13)	0.0260 (12)	0.0097 (10)	0.0059 (9)	0.0083 (10)
C203	0.0242 (12)	0.0547 (16)	0.0233 (12)	0.0142 (11)	0.0008 (9)	0.0049 (11)
C204	0.0522 (17)	0.0472 (16)	0.0201 (12)	0.0306 (14)	−0.0077 (11)	−0.0023 (11)
C205	0.087 (2)	0.0292 (14)	0.0390 (16)	0.0194 (15)	−0.0252 (16)	0.0006 (12)
C206	0.068 (2)	0.0262 (13)	0.0385 (15)	0.0109 (13)	−0.0240 (14)	−0.0005 (11)
C211	0.0218 (10)	0.0179 (10)	0.0167 (10)	0.0046 (8)	0.0030 (8)	−0.0007 (8)
C212	0.0213 (10)	0.0286 (11)	0.0182 (10)	0.0086 (9)	0.0010 (8)	−0.0008 (9)
C213	0.0251 (11)	0.0379 (13)	0.0172 (10)	0.0086 (10)	0.0015 (9)	−0.0049 (9)
C214	0.0243 (11)	0.0294 (12)	0.0244 (11)	0.0094 (9)	0.0063 (9)	−0.0059 (9)
C215	0.0223 (11)	0.0251 (11)	0.0261 (11)	0.0084 (9)	−0.0007 (9)	−0.0001 (9)
C216	0.0282 (11)	0.0234 (11)	0.0163 (10)	0.0062 (9)	−0.0008 (8)	−0.0004 (8)
C221	0.0188 (10)	0.0240 (11)	0.0168 (10)	0.0060 (8)	−0.0026 (8)	0.0024 (8)
C222	0.0239 (11)	0.0253 (11)	0.0267 (12)	0.0076 (9)	0.0018 (9)	0.0003 (9)
C223	0.0251 (12)	0.0246 (11)	0.0371 (13)	0.0041 (9)	−0.0017 (10)	0.0033 (10)
C224	0.0226 (11)	0.0387 (13)	0.0282 (12)	−0.0037 (10)	−0.0036 (9)	0.0070 (10)
C225	0.0272 (12)	0.0447 (15)	0.0219 (11)	−0.0023 (11)	0.0038 (9)	−0.0039 (10)
C226	0.0289 (12)	0.0317 (12)	0.0219 (11)	0.0003 (10)	0.0029 (9)	−0.0056 (9)

Geometric parameters (Å, º)

Mn1—C16	1.768 (2)	Mn2—C27	1.768 (2)
Mn1—C17	1.776 (2)	Mn2—C26	1.776 (2)
Mn1—C15	2.127 (2)	Mn2—C21	2.142 (2)
Mn1—C14	2.132 (2)	Mn2—C24	2.143 (3)
Mn1—C11	2.153 (2)	Mn2—C25	2.146 (2)
Mn1—C13	2.157 (2)	Mn2—C22	2.150 (2)
Mn1—C12	2.162 (2)	Mn2—C23	2.151 (2)
Mn1—P1	2.2259 (6)	Mn2—P2	2.2421 (7)
P1—C121	1.833 (2)	P2—C211	1.836 (2)
P1—C111	1.837 (2)	P2—C201	1.837 (2)
P1—C101	1.843 (2)	P2—C221	1.842 (2)
C11—C12	1.414 (3)	C21—C25	1.404 (4)
C11—C15	1.419 (3)	C21—C22	1.416 (4)
C11—H11	0.9500	C21—H21	0.9500
C12—C13	1.412 (3)	C22—C23	1.418 (4)

C12—H12	0.9500	C22—H22	0.9500
C13—C14	1.421 (4)	C23—C24	1.412 (4)
C13—H13	0.9500	C23—H23	0.9500
C14—C15	1.409 (4)	C24—C25	1.421 (4)
C14—H14	0.9500	C24—H24	0.9500
C15—H15	0.9500	C25—H25	0.9500
C16—O11	1.165 (3)	C26—O21	1.162 (3)
C17—O12	1.162 (3)	C27—O22	1.159 (3)
C101—C106	1.395 (3)	C201—C202	1.389 (3)
C101—C102	1.400 (3)	C201—C206	1.391 (4)
C102—C103	1.387 (3)	C202—C203	1.393 (3)
C102—H102	0.9500	C202—H202	0.9500
C103—C104	1.387 (3)	C203—C204	1.381 (4)
C103—H103	0.9500	C203—H203	0.9500
C104—C105	1.382 (3)	C204—C205	1.382 (4)
C104—H104	0.9500	C204—H204	0.9500
C105—C106	1.394 (3)	C205—C206	1.395 (4)
C105—H105	0.9500	C205—H205	0.9500
C106—H106	0.9500	C206—H206	0.9500
C111—C112	1.391 (3)	C211—C212	1.392 (3)
C111—C116	1.397 (3)	C211—C216	1.398 (3)
C112—C113	1.393 (3)	C212—C213	1.392 (3)
C112—H112	0.9500	C212—H212	0.9500
C113—C114	1.383 (4)	C213—C214	1.384 (3)
C113—H113	0.9500	C213—H213	0.9500
C114—C115	1.384 (3)	C214—C215	1.386 (3)
C114—H114	0.9500	C214—H214	0.9500
C115—C116	1.386 (3)	C215—C216	1.382 (3)
C115—H115	0.9500	C215—H215	0.9500
C116—H116	0.9500	C216—H216	0.9500
C121—C122	1.391 (3)	C221—C226	1.396 (3)
C121—C126	1.395 (3)	C221—C222	1.397 (3)
C122—C123	1.389 (3)	C222—C223	1.390 (3)
C122—H122	0.9500	C222—H222	0.9500
C123—C124	1.380 (3)	C223—C224	1.382 (3)
C123—H123	0.9500	C223—H223	0.9500
C124—C125	1.384 (3)	C224—C225	1.383 (4)
C124—H124	0.9500	C224—H224	0.9500
C125—C126	1.389 (3)	C225—C226	1.388 (3)
C125—H125	0.9500	C225—H225	0.9500
C126—H126	0.9500	C226—H226	0.9500
C16—Mn1—C17	92.56 (11)	C27—Mn2—C26	92.40 (10)
C16—Mn1—C15	89.43 (10)	C27—Mn2—C21	136.46 (10)
C17—Mn1—C15	125.40 (10)	C26—Mn2—C21	130.93 (10)
C16—Mn1—C14	114.54 (10)	C27—Mn2—C24	90.25 (10)
C17—Mn1—C14	93.58 (10)	C26—Mn2—C24	123.47 (10)
C15—Mn1—C14	38.63 (9)	C21—Mn2—C24	64.39 (11)

C16—Mn1—C11	101.41 (9)	C27—Mn2—C25	100.11 (10)
C17—Mn1—C11	157.66 (10)	C26—Mn2—C25	157.44 (10)
C15—Mn1—C11	38.71 (9)	C21—Mn2—C25	38.22 (10)
C14—Mn1—C11	64.82 (9)	C24—Mn2—C25	38.70 (10)
C16—Mn1—C13	152.38 (10)	C27—Mn2—C22	153.93 (11)
C17—Mn1—C13	95.54 (10)	C26—Mn2—C22	96.74 (10)
C15—Mn1—C13	64.45 (9)	C21—Mn2—C22	38.52 (10)
C14—Mn1—C13	38.68 (10)	C24—Mn2—C22	64.38 (11)
C11—Mn1—C13	64.31 (9)	C25—Mn2—C22	64.34 (10)
C16—Mn1—C12	138.51 (9)	C27—Mn2—C23	116.83 (10)
C17—Mn1—C12	128.62 (11)	C26—Mn2—C23	93.13 (10)
C15—Mn1—C12	64.26 (9)	C21—Mn2—C23	64.45 (10)
C14—Mn1—C12	64.43 (9)	C24—Mn2—C23	38.37 (10)
C11—Mn1—C12	38.25 (8)	C25—Mn2—C23	64.49 (10)
C13—Mn1—C12	38.17 (9)	C22—Mn2—C23	38.50 (10)
C16—Mn1—P1	89.83 (7)	C27—Mn2—P2	91.14 (7)
C17—Mn1—P1	93.44 (7)	C26—Mn2—P2	93.87 (8)
C15—Mn1—P1	141.14 (7)	C21—Mn2—P2	89.93 (8)
C14—Mn1—P1	154.26 (8)	C24—Mn2—P2	142.54 (7)
C11—Mn1—P1	103.85 (6)	C25—Mn2—P2	104.49 (7)
C13—Mn1—P1	115.90 (7)	C22—Mn2—P2	112.44 (8)
C12—Mn1—P1	92.10 (6)	C23—Mn2—P2	150.81 (7)
C121—P1—C111	103.65 (9)	C211—P2—C201	102.14 (9)
C121—P1—C101	100.81 (9)	C211—P2—C221	102.08 (10)
C111—P1—C101	101.61 (9)	C201—P2—C221	101.53 (10)
C121—P1—Mn1	119.18 (7)	C211—P2—Mn2	112.82 (7)
C111—P1—Mn1	114.28 (7)	C201—P2—Mn2	118.37 (8)
C101—P1—Mn1	114.95 (7)	C221—P2—Mn2	117.52 (7)
C12—C11—C15	107.3 (2)	C25—C21—C22	108.4 (2)
C12—C11—Mn1	71.24 (12)	C25—C21—Mn2	71.03 (14)
C15—C11—Mn1	69.66 (12)	C22—C21—Mn2	71.04 (14)
C12—C11—H11	126.3	C25—C21—H21	125.8
C15—C11—H11	126.3	C22—C21—H21	125.8
Mn1—C11—H11	124.4	Mn2—C21—H21	123.8
C13—C12—C11	108.5 (2)	C21—C22—C23	107.8 (2)
C13—C12—Mn1	70.71 (13)	C21—C22—Mn2	70.44 (13)
C11—C12—Mn1	70.51 (12)	C23—C22—Mn2	70.79 (14)
C13—C12—H12	125.7	C21—C22—H22	126.1
C11—C12—H12	125.7	C23—C22—H22	126.1
Mn1—C12—H12	124.6	Mn2—C22—H22	124.3
C12—C13—C14	107.8 (2)	C24—C23—C22	107.9 (2)
C12—C13—Mn1	71.13 (13)	C24—C23—Mn2	70.50 (14)
C14—C13—Mn1	69.71 (14)	C22—C23—Mn2	70.70 (14)
C12—C13—H13	126.1	C24—C23—H23	126.1
C14—C13—H13	126.1	C22—C23—H23	126.1
Mn1—C13—H13	124.7	Mn2—C23—H23	124.3
C15—C14—C13	107.7 (2)	C23—C24—C25	108.1 (2)
C15—C14—Mn1	70.49 (13)	C23—C24—Mn2	71.12 (15)

C13—C14—Mn1	71.60 (13)	C25—C24—Mn2	70.76 (14)
C15—C14—H14	126.2	C23—C24—H24	126.0
C13—C14—H14	126.2	C25—C24—H24	126.0
Mn1—C14—H14	123.4	Mn2—C24—H24	123.8
C14—C15—C11	108.6 (2)	C21—C25—C24	107.9 (2)
C14—C15—Mn1	70.89 (13)	C21—C25—Mn2	70.75 (14)
C11—C15—Mn1	71.63 (12)	C24—C25—Mn2	70.54 (14)
C14—C15—H15	125.7	C21—C25—H25	126.1
C11—C15—H15	125.7	C24—C25—H25	126.1
Mn1—C15—H15	123.4	Mn2—C25—H25	124.3
O11—C16—Mn1	177.06 (19)	O21—C26—Mn2	176.3 (2)
O12—C17—Mn1	175.7 (2)	O22—C27—Mn2	176.7 (2)
C106—C101—C102	118.11 (19)	C202—C201—C206	118.7 (2)
C106—C101—P1	123.19 (16)	C202—C201—P2	122.21 (18)
C102—C101—P1	118.67 (15)	C206—C201—P2	118.95 (19)
C103—C102—C101	120.9 (2)	C201—C202—C203	120.7 (2)
C103—C102—H102	119.5	C201—C202—H202	119.6
C101—C102—H102	119.5	C203—C202—H202	119.6
C102—C103—C104	120.3 (2)	C204—C203—C202	119.8 (3)
C102—C103—H103	119.8	C204—C203—H203	120.1
C104—C103—H103	119.8	C202—C203—H203	120.1
C105—C104—C103	119.5 (2)	C203—C204—C205	120.4 (2)
C105—C104—H104	120.3	C203—C204—H204	119.8
C103—C104—H104	120.3	C205—C204—H204	119.8
C104—C105—C106	120.4 (2)	C204—C205—C206	119.6 (3)
C104—C105—H105	119.8	C204—C205—H205	120.2
C106—C105—H105	119.8	C206—C205—H205	120.2
C105—C106—C101	120.8 (2)	C201—C206—C205	120.8 (3)
C105—C106—H106	119.6	C201—C206—H206	119.6
C101—C106—H106	119.6	C205—C206—H206	119.6
C112—C111—C116	118.38 (19)	C212—C211—C216	118.87 (19)
C112—C111—P1	123.56 (16)	C212—C211—P2	122.99 (16)
C116—C111—P1	117.99 (15)	C216—C211—P2	118.12 (16)
C111—C112—C113	120.3 (2)	C211—C212—C213	120.3 (2)
C111—C112—H112	119.8	C211—C212—H212	119.9
C113—C112—H112	119.8	C213—C212—H212	119.9
C114—C113—C112	120.6 (2)	C214—C213—C212	120.2 (2)
C114—C113—H113	119.7	C214—C213—H213	119.9
C112—C113—H113	119.7	C212—C213—H213	119.9
C113—C114—C115	119.6 (2)	C213—C214—C215	119.8 (2)
C113—C114—H114	120.2	C213—C214—H214	120.1
C115—C114—H114	120.2	C215—C214—H214	120.1
C114—C115—C116	120.0 (2)	C216—C215—C214	120.1 (2)
C114—C115—H115	120.0	C216—C215—H215	120.0
C116—C115—H115	120.0	C214—C215—H215	120.0
C115—C116—C111	121.1 (2)	C215—C216—C211	120.7 (2)
C115—C116—H116	119.5	C215—C216—H216	119.7
C111—C116—H116	119.5	C211—C216—H216	119.7

C122—C121—C126	118.62 (19)	C226—C221—C222	117.7 (2)
C122—C121—P1	120.31 (16)	C226—C221—P2	119.31 (17)
C126—C121—P1	121.07 (16)	C222—C221—P2	122.97 (17)
C123—C122—C121	120.4 (2)	C223—C222—C221	121.0 (2)
C123—C122—H122	119.8	C223—C222—H222	119.5
C121—C122—H122	119.8	C221—C222—H222	119.5
C124—C123—C122	120.5 (2)	C224—C223—C222	120.3 (2)
C124—C123—H123	119.7	C224—C223—H223	119.8
C122—C123—H123	119.7	C222—C223—H223	119.8
C123—C124—C125	119.7 (2)	C223—C224—C225	119.3 (2)
C123—C124—H124	120.1	C223—C224—H224	120.3
C125—C124—H124	120.1	C225—C224—H224	120.3
C124—C125—C126	119.9 (2)	C224—C225—C226	120.5 (2)
C124—C125—H125	120.0	C224—C225—H225	119.8
C126—C125—H125	120.0	C226—C225—H225	119.8
C125—C126—C121	120.8 (2)	C225—C226—C221	121.1 (2)
C125—C126—H126	119.6	C225—C226—H226	119.5
C121—C126—H126	119.6	C221—C226—H226	119.5
C15—C11—C12—C13	0.2 (2)	C25—C21—C22—C23	0.3 (3)
Mn1—C11—C12—C13	60.78 (15)	Mn2—C21—C22—C23	−61.28 (18)
C15—C11—C12—Mn1	−60.63 (14)	C25—C21—C22—Mn2	61.53 (17)
C11—C12—C13—C14	−0.3 (3)	C21—C22—C23—C24	0.0 (3)
Mn1—C12—C13—C14	60.33 (16)	Mn2—C22—C23—C24	−61.03 (17)
C11—C12—C13—Mn1	−60.66 (15)	C21—C22—C23—Mn2	61.05 (18)
C12—C13—C14—C15	0.4 (3)	C22—C23—C24—C25	−0.3 (3)
Mn1—C13—C14—C15	61.61 (16)	Mn2—C23—C24—C25	−61.44 (17)
C12—C13—C14—Mn1	−61.23 (15)	C22—C23—C24—Mn2	61.16 (18)
C13—C14—C15—C11	−0.3 (3)	C22—C21—C25—C24	−0.4 (3)
Mn1—C14—C15—C11	62.04 (15)	Mn2—C21—C25—C24	61.11 (16)
C13—C14—C15—Mn1	−62.33 (16)	C22—C21—C25—Mn2	−61.53 (18)
C12—C11—C15—C14	0.1 (2)	C23—C24—C25—C21	0.4 (3)
Mn1—C11—C15—C14	−61.57 (15)	Mn2—C24—C25—C21	−61.24 (17)
C12—C11—C15—Mn1	61.65 (15)	C23—C24—C25—Mn2	61.68 (17)
C121—P1—C101—C106	119.77 (18)	C211—P2—C201—C202	−72.7 (2)
C111—P1—C101—C106	13.2 (2)	C221—P2—C201—C202	32.5 (2)
Mn1—P1—C101—C106	−110.72 (17)	Mn2—P2—C201—C202	162.74 (16)
C121—P1—C101—C102	−62.04 (17)	C211—P2—C201—C206	103.2 (2)
C111—P1—C101—C102	−168.57 (16)	C221—P2—C201—C206	−151.6 (2)
Mn1—P1—C101—C102	67.47 (17)	Mn2—P2—C201—C206	−21.3 (2)
C106—C101—C102—C103	0.6 (3)	C206—C201—C202—C203	0.1 (4)
P1—C101—C102—C103	−177.73 (16)	P2—C201—C202—C203	176.02 (18)
C101—C102—C103—C104	0.0 (3)	C201—C202—C203—C204	−0.6 (4)
C102—C103—C104—C105	−0.4 (3)	C202—C203—C204—C205	0.0 (4)
C103—C104—C105—C106	0.2 (3)	C203—C204—C205—C206	1.1 (5)
C104—C105—C106—C101	0.4 (3)	C202—C201—C206—C205	1.0 (4)
C102—C101—C106—C105	−0.8 (3)	P2—C201—C206—C205	−175.1 (3)
P1—C101—C106—C105	177.44 (17)	C204—C205—C206—C201	−1.6 (5)

C121—P1—C111—C112	−4.7 (2)	C201—P2—C211—C212	−2.2 (2)
C101—P1—C111—C112	99.60 (18)	C221—P2—C211—C212	−107.0 (2)
Mn1—P1—C111—C112	−135.99 (16)	Mn2—P2—C211—C212	125.97 (18)
C121—P1—C111—C116	178.39 (16)	C201—P2—C211—C216	179.22 (18)
C101—P1—C111—C116	−77.32 (17)	C221—P2—C211—C216	74.44 (19)
Mn1—P1—C111—C116	47.10 (17)	Mn2—P2—C211—C216	−52.62 (19)
C116—C111—C112—C113	2.9 (3)	C216—C211—C212—C213	−0.7 (3)
P1—C111—C112—C113	−174.03 (17)	P2—C211—C212—C213	−179.25 (18)
C111—C112—C113—C114	−0.2 (3)	C211—C212—C213—C214	0.4 (4)
C112—C113—C114—C115	−2.3 (3)	C212—C213—C214—C215	−0.3 (4)
C113—C114—C115—C116	2.0 (3)	C213—C214—C215—C216	0.5 (4)
C114—C115—C116—C111	0.7 (3)	C214—C215—C216—C211	−0.8 (4)
C112—C111—C116—C115	−3.2 (3)	C212—C211—C216—C215	0.9 (3)
P1—C111—C116—C115	173.92 (16)	P2—C211—C216—C215	179.51 (18)
C111—P1—C121—C122	−112.90 (18)	C211—P2—C221—C226	−174.52 (17)
C101—P1—C121—C122	142.20 (17)	C201—P2—C221—C226	80.23 (19)
Mn1—P1—C121—C122	15.4 (2)	Mn2—P2—C221—C226	−50.55 (19)
C111—P1—C121—C126	66.33 (19)	C211—P2—C221—C222	7.3 (2)
C101—P1—C121—C126	−38.58 (19)	C201—P2—C221—C222	−98.00 (19)
Mn1—P1—C121—C126	−165.34 (14)	Mn2—P2—C221—C222	131.22 (17)
C126—C121—C122—C123	−1.0 (3)	C226—C221—C222—C223	0.8 (3)
P1—C121—C122—C123	178.22 (17)	P2—C221—C222—C223	179.04 (17)
C121—C122—C123—C124	1.2 (3)	C221—C222—C223—C224	−1.7 (3)
C122—C123—C124—C125	−0.6 (3)	C222—C223—C224—C225	1.2 (4)
C123—C124—C125—C126	−0.2 (3)	C223—C224—C225—C226	0.2 (4)
C124—C125—C126—C121	0.4 (3)	C224—C225—C226—C221	−1.1 (4)
C122—C121—C126—C125	0.2 (3)	C222—C221—C226—C225	0.6 (3)
P1—C121—C126—C125	−179.01 (17)	P2—C221—C226—C225	−177.74 (18)

Dicarbonyl(η^5-1-chlorocyclopentadienyl)(triphenylphosphane-κP)manganese(I) (compd1b)

Crystal data

[Mn(C$_5$H$_4$Cl)(C$_{18}$H$_{15}$P)(CO)$_2$]	$D_x = 1.457$ Mg m^{-3}
$M_r = 472.76$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 3646 reflections
$a = 7.6519$ (3) Å	$\theta = 4.6$–27.6°
$b = 16.4786$ (7) Å	$\mu = 0.83$ mm^{-1}
$c = 17.0971$ (7) Å	$T = 173$ K
$V = 2155.82$ (15) Å^3	Block, yellow
$Z = 4$	0.34 × 0.14 × 0.10 mm
$F(000) = 968$	

Data collection

Oxford Diffraction KM4 Xcalibur2 diffractometer	14524 measured reflections
	4900 independent reflections
Radiation source: Enhance (Mo) X-ray Source	4297 reflections with $I > 2\sigma(I)$
Detector resolution: 15.9809 pixels mm^{-1}	$R_{int} = 0.045$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 4.4°$
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)	$h = -9 \rightarrow 9$
	$k = -20 \rightarrow 21$
$T_{min} = 0.892$, $T_{max} = 1$	$l = -22 \rightarrow 21$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.3065P]$
$R[F^2 > 2\sigma(F^2)] = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.082$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.39$ e Å^{-3}
4900 reflections	$\Delta\rho_{min} = -0.29$ e Å^{-3}
271 parameters	Absolute structure: Flack x determined using
0 restraints	1609 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et*
Primary atom site location: dual	*al.*, 2013)
Hydrogen site location: inferred from	Absolute structure parameter: −0.038 (12)
neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
C1	0.7487 (5)	0.3166 (2)	0.3742 (2)	0.0300 (9)
C2	0.8076 (6)	0.3768 (3)	0.3225 (2)	0.0335 (9)
H2	0.772105	0.383858	0.269734	0.040*
C3	0.9300 (5)	0.4253 (3)	0.3637 (2)	0.0349 (9)
H3	0.991787	0.470731	0.343659	0.042*
C4	0.9429 (5)	0.3934 (3)	0.4402 (2)	0.0350 (10)
H4	1.015964	0.413982	0.480477	0.042*
C5	0.8308 (5)	0.3265 (2)	0.4471 (2)	0.0322 (9)
H5	0.813499	0.294159	0.492436	0.039*
C6	0.4855 (5)	0.3976 (2)	0.4648 (2)	0.0250 (8)
C7	0.7072 (5)	0.5105 (2)	0.4929 (2)	0.0284 (8)
C11	0.3820 (5)	0.4804 (2)	0.2738 (2)	0.0222 (7)
C12	0.2759 (5)	0.5304 (2)	0.2289 (2)	0.0279 (8)
H12	0.281137	0.587602	0.235804	0.033*
C13	0.1618 (5)	0.4976 (3)	0.1737 (2)	0.0351 (10)
H13	0.090675	0.532439	0.143004	0.042*
C14	0.1518 (5)	0.4151 (3)	0.1636 (2)	0.0389 (10)
H14	0.075065	0.392769	0.125577	0.047*
C15	0.2539 (6)	0.3648 (3)	0.2090 (3)	0.0402 (11)
H15	0.245968	0.307662	0.202826	0.048*
C16	0.3683 (5)	0.3972 (2)	0.2638 (2)	0.0328 (9)
H16	0.437971	0.361861	0.294715	0.039*
C21	0.4127 (5)	0.6032 (2)	0.3891 (2)	0.0231 (8)
C22	0.4289 (5)	0.6840 (2)	0.3676 (2)	0.0276 (8)
H22	0.511604	0.698829	0.328666	0.033*
C23	0.3256 (6)	0.7435 (2)	0.4021 (2)	0.0359 (9)
H23	0.339365	0.798696	0.387320	0.043*
C24	0.2036 (6)	0.7226 (3)	0.4578 (2)	0.0390 (11)

H24	0.133723	0.763252	0.481678	0.047*
C25	0.1833 (6)	0.6419 (3)	0.4787 (2)	0.0416 (11)
H25	0.097627	0.627007	0.516304	0.050*
C26	0.2875 (5)	0.5831 (3)	0.4451 (2)	0.0360 (10)
H26	0.273599	0.527996	0.460334	0.043*
C31	0.6917 (5)	0.5794 (2)	0.28135 (19)	0.0220 (7)
C32	0.8238 (5)	0.6237 (2)	0.3178 (2)	0.0279 (8)
H32	0.836357	0.621350	0.372994	0.033*
C33	0.9372 (5)	0.6711 (2)	0.2740 (3)	0.0349 (9)
H33	1.026664	0.701044	0.299401	0.042*
C34	0.9208 (5)	0.6749 (3)	0.1936 (2)	0.0375 (10)
H34	0.996460	0.708650	0.163827	0.045*
C35	0.7941 (5)	0.6297 (2)	0.1570 (2)	0.0349 (9)
H35	0.784854	0.631243	0.101653	0.042*
C36	0.6785 (5)	0.5813 (2)	0.1999 (2)	0.0262 (8)
H36	0.591887	0.550077	0.173838	0.031*
Cl1	0.61091 (16)	0.23638 (6)	0.35295 (7)	0.0463 (3)
Mn1	0.68106 (7)	0.43367 (3)	0.42154 (3)	0.02044 (13)
O1	0.3631 (4)	0.37057 (18)	0.49453 (17)	0.0403 (7)
O2	0.7294 (4)	0.55948 (19)	0.54096 (16)	0.0440 (8)
P1	0.54153 (12)	0.52133 (5)	0.34323 (5)	0.0200 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.031 (2)	0.024 (2)	0.035 (2)	0.0097 (16)	0.0046 (18)	−0.0063 (16)
C2	0.029 (2)	0.042 (2)	0.029 (2)	0.0136 (19)	0.0086 (19)	−0.0036 (17)
C3	0.0229 (19)	0.037 (2)	0.045 (2)	0.0072 (17)	0.0106 (18)	0.0058 (19)
C4	0.023 (2)	0.039 (2)	0.042 (3)	0.0101 (17)	−0.0052 (18)	−0.0030 (18)
C5	0.035 (2)	0.028 (2)	0.033 (2)	0.0105 (18)	0.0023 (19)	0.0030 (16)
C6	0.030 (2)	0.0206 (19)	0.0247 (19)	0.0038 (16)	−0.0008 (16)	0.0055 (15)
C7	0.030 (2)	0.026 (2)	0.0287 (19)	−0.0003 (16)	−0.0008 (17)	0.0056 (16)
C11	0.0207 (17)	0.0239 (18)	0.0221 (17)	−0.0007 (14)	0.0031 (15)	0.0019 (15)
C12	0.027 (2)	0.0225 (19)	0.034 (2)	0.0024 (15)	−0.0025 (17)	−0.0009 (16)
C13	0.031 (2)	0.042 (3)	0.032 (2)	0.0039 (19)	−0.0107 (19)	0.0035 (17)
C14	0.035 (2)	0.049 (3)	0.033 (2)	−0.0022 (19)	−0.0087 (19)	−0.0097 (18)
C15	0.045 (3)	0.025 (2)	0.051 (3)	−0.0021 (18)	−0.009 (2)	−0.0058 (19)
C16	0.034 (2)	0.026 (2)	0.039 (2)	0.0018 (17)	−0.0087 (19)	0.0023 (17)
C21	0.0225 (19)	0.0245 (19)	0.0224 (18)	0.0020 (14)	−0.0009 (15)	−0.0005 (14)
C22	0.027 (2)	0.027 (2)	0.028 (2)	0.0010 (15)	0.0003 (16)	−0.0019 (15)
C23	0.038 (2)	0.027 (2)	0.043 (2)	0.0061 (18)	−0.007 (2)	−0.0065 (17)
C24	0.040 (2)	0.044 (3)	0.032 (2)	0.018 (2)	−0.001 (2)	−0.0110 (18)
C25	0.039 (2)	0.051 (3)	0.035 (2)	0.015 (2)	0.013 (2)	0.0042 (19)
C26	0.034 (2)	0.035 (2)	0.038 (2)	0.0059 (18)	0.0100 (18)	0.0083 (17)
C31	0.0212 (17)	0.0212 (19)	0.0236 (17)	0.0026 (15)	0.0055 (15)	0.0023 (14)
C32	0.0247 (19)	0.028 (2)	0.0313 (19)	0.0007 (16)	−0.0032 (18)	0.0003 (15)
C33	0.030 (2)	0.026 (2)	0.049 (3)	−0.0054 (17)	0.003 (2)	0.0012 (18)
C34	0.034 (2)	0.035 (2)	0.043 (2)	−0.0071 (18)	0.015 (2)	0.0122 (19)

C35	0.037 (2)	0.041 (2)	0.027 (2)	0.0031 (19)	0.0104 (19)	0.0064 (17)
C36	0.0244 (18)	0.030 (2)	0.0245 (17)	−0.0037 (16)	0.0011 (16)	0.0002 (14)
Cl1	0.0535 (7)	0.0266 (5)	0.0587 (7)	0.0037 (5)	−0.0085 (6)	−0.0096 (5)
Mn1	0.0205 (3)	0.0196 (3)	0.0212 (2)	0.0019 (2)	0.0011 (2)	0.0011 (2)
O1	0.0332 (17)	0.0362 (17)	0.0515 (18)	−0.0017 (13)	0.0118 (14)	0.0140 (14)
O2	0.058 (2)	0.0349 (17)	0.0394 (16)	−0.0031 (15)	−0.0052 (15)	−0.0121 (14)
P1	0.0199 (5)	0.0193 (4)	0.0209 (4)	0.0005 (4)	0.0013 (4)	0.0012 (4)

Geometric parameters (Å, º)

C1—C2	1.402 (6)	C15—C16	1.388 (6)
C1—C5	1.406 (5)	C15—H15	0.9500
C1—Cl1	1.730 (4)	C16—H16	0.9500
C1—Mn1	2.155 (4)	C21—C22	1.387 (5)
C2—C3	1.418 (6)	C21—C26	1.394 (5)
C2—Mn1	2.163 (4)	C21—P1	1.846 (4)
C2—H2	0.9500	C22—C23	1.392 (5)
C3—C4	1.412 (6)	C22—H22	0.9500
C3—Mn1	2.150 (4)	C23—C24	1.377 (6)
C3—H3	0.9500	C23—H23	0.9500
C4—C5	1.401 (6)	C24—C25	1.386 (6)
C4—Mn1	2.135 (4)	C24—H24	0.9500
C4—H4	0.9500	C25—C26	1.380 (6)
C5—Mn1	2.149 (4)	C25—H25	0.9500
C5—H5	0.9500	C26—H26	0.9500
C6—O1	1.154 (4)	C31—C32	1.394 (5)
C6—Mn1	1.772 (4)	C31—C36	1.397 (5)
C7—O2	1.163 (5)	C31—P1	1.832 (3)
C7—Mn1	1.770 (4)	C32—C33	1.387 (5)
C11—C16	1.386 (5)	C32—H32	0.9500
C11—C12	1.389 (5)	C33—C34	1.382 (6)
C11—P1	1.831 (4)	C33—H33	0.9500
C12—C13	1.395 (5)	C34—C35	1.374 (6)
C12—H12	0.9500	C34—H34	0.9500
C13—C14	1.373 (6)	C35—C36	1.397 (5)
C13—H13	0.9500	C35—H35	0.9500
C14—C15	1.378 (6)	C36—H36	0.9500
C14—H14	0.9500	Mn1—P1	2.2403 (10)
C2—C1—C5	109.4 (4)	C23—C24—H24	120.2
C2—C1—Cl1	127.2 (3)	C25—C24—H24	120.2
C5—C1—Cl1	123.2 (3)	C26—C25—C24	120.1 (4)
C2—C1—Mn1	71.4 (2)	C26—C25—H25	120.0
C5—C1—Mn1	70.7 (2)	C24—C25—H25	120.0
Cl1—C1—Mn1	128.1 (2)	C25—C26—C21	121.1 (4)
C1—C2—C3	107.3 (4)	C25—C26—H26	119.5
C1—C2—Mn1	70.7 (2)	C21—C26—H26	119.5
C3—C2—Mn1	70.3 (2)	C32—C31—C36	119.1 (3)

C1—C2—H2	126.3	C32—C31—P1	118.1 (3)
C3—C2—H2	126.3	C36—C31—P1	122.9 (3)
Mn1—C2—H2	124.2	C33—C32—C31	120.5 (3)
C4—C3—C2	107.2 (4)	C33—C32—H32	119.8
C4—C3—Mn1	70.2 (2)	C31—C32—H32	119.8
C2—C3—Mn1	71.3 (2)	C34—C33—C32	120.4 (4)
C4—C3—H3	126.4	C34—C33—H33	119.8
C2—C3—H3	126.4	C32—C33—H33	119.8
Mn1—C3—H3	123.8	C35—C34—C33	119.4 (4)
C5—C4—C3	109.2 (4)	C35—C34—H34	120.3
C5—C4—Mn1	71.5 (2)	C33—C34—H34	120.3
C3—C4—Mn1	71.4 (2)	C34—C35—C36	121.2 (4)
C5—C4—H4	125.4	C34—C35—H35	119.4
C3—C4—H4	125.4	C36—C35—H35	119.4
Mn1—C4—H4	123.3	C31—C36—C35	119.3 (4)
C4—C5—C1	106.8 (4)	C31—C36—H36	120.3
C4—C5—Mn1	70.3 (2)	C35—C36—H36	120.3
C1—C5—Mn1	71.2 (2)	C7—Mn1—C6	92.72 (17)
C4—C5—H5	126.6	C7—Mn1—C4	90.78 (17)
C1—C5—H5	126.6	C6—Mn1—C4	128.76 (16)
Mn1—C5—H5	123.6	C7—Mn1—C5	112.78 (16)
O1—C6—Mn1	176.3 (3)	C6—Mn1—C5	95.14 (17)
O2—C7—Mn1	177.5 (4)	C4—Mn1—C5	38.18 (16)
C16—C11—C12	118.3 (4)	C7—Mn1—C3	105.24 (17)
C16—C11—P1	119.7 (3)	C6—Mn1—C3	156.69 (16)
C12—C11—P1	122.0 (3)	C4—Mn1—C3	38.48 (16)
C11—C12—C13	120.6 (4)	C5—Mn1—C3	64.44 (16)
C11—C12—H12	119.7	C7—Mn1—C1	150.74 (16)
C13—C12—H12	119.7	C6—Mn1—C1	93.42 (16)
C14—C13—C12	120.3 (4)	C4—Mn1—C1	63.40 (16)
C14—C13—H13	119.8	C5—Mn1—C1	38.13 (15)
C12—C13—H13	119.8	C3—Mn1—C1	63.70 (16)
C13—C14—C15	119.5 (4)	C7—Mn1—C2	143.00 (18)
C13—C14—H14	120.3	C6—Mn1—C2	124.02 (17)
C15—C14—H14	120.3	C4—Mn1—C2	64.02 (16)
C14—C15—C16	120.5 (4)	C5—Mn1—C2	64.21 (15)
C14—C15—H15	119.8	C3—Mn1—C2	38.38 (16)
C16—C15—H15	119.8	C1—Mn1—C2	37.89 (15)
C11—C16—C15	120.7 (4)	C7—Mn1—P1	90.26 (12)
C11—C16—H16	119.6	C6—Mn1—P1	93.63 (12)
C15—C16—H16	119.6	C4—Mn1—P1	137.48 (12)
C22—C21—C26	118.2 (4)	C5—Mn1—P1	154.84 (11)
C22—C21—P1	122.7 (3)	C3—Mn1—P1	100.89 (11)
C26—C21—P1	119.0 (3)	C1—Mn1—P1	117.83 (11)
C21—C22—C23	120.9 (4)	C2—Mn1—P1	91.43 (11)
C21—C22—H22	119.6	C11—P1—C31	103.68 (16)
C23—C22—H22	119.6	C11—P1—C21	100.86 (16)
C24—C23—C22	120.1 (4)	C31—P1—C21	101.48 (16)

C24—C23—H23	119.9	C11—P1—Mn1	117.87 (12)
C22—C23—H23	119.9	C31—P1—Mn1	112.51 (12)
C23—C24—C25	119.7 (4)	C21—P1—Mn1	118.14 (12)
C5—C1—C2—C3	0.4 (4)	C23—C24—C25—C26	1.3 (7)
Cl1—C1—C2—C3	−174.8 (3)	C24—C25—C26—C21	−0.8 (7)
Mn1—C1—C2—C3	61.1 (3)	C22—C21—C26—C25	−0.5 (6)
C5—C1—C2—Mn1	−60.7 (3)	P1—C21—C26—C25	−177.4 (3)
Cl1—C1—C2—Mn1	124.1 (3)	C36—C31—C32—C33	2.0 (5)
C1—C2—C3—C4	−0.1 (4)	P1—C31—C32—C33	−177.6 (3)
Mn1—C2—C3—C4	61.3 (3)	C31—C32—C33—C34	−0.1 (6)
C1—C2—C3—Mn1	−61.4 (3)	C32—C33—C34—C35	−1.8 (6)
C2—C3—C4—C5	−0.2 (4)	C33—C34—C35—C36	1.7 (6)
Mn1—C3—C4—C5	61.8 (3)	C32—C31—C36—C35	−2.2 (5)
C2—C3—C4—Mn1	−62.1 (3)	P1—C31—C36—C35	177.5 (3)
C3—C4—C5—C1	0.4 (4)	C34—C35—C36—C31	0.3 (6)
Mn1—C4—C5—C1	62.2 (3)	C16—C11—P1—C31	116.4 (3)
C3—C4—C5—Mn1	−61.8 (3)	C12—C11—P1—C31	−61.9 (3)
C2—C1—C5—C4	−0.5 (4)	C16—C11—P1—C21	−138.8 (3)
Cl1—C1—C5—C4	174.9 (3)	C12—C11—P1—C21	42.9 (3)
Mn1—C1—C5—C4	−61.7 (3)	C16—C11—P1—Mn1	−8.7 (4)
C2—C1—C5—Mn1	61.2 (3)	C12—C11—P1—Mn1	173.0 (3)
Cl1—C1—C5—Mn1	−123.5 (3)	C32—C31—P1—C11	175.5 (3)
C16—C11—C12—C13	−1.6 (6)	C36—C31—P1—C11	−4.1 (3)
P1—C11—C12—C13	176.8 (3)	C32—C31—P1—C21	71.2 (3)
C11—C12—C13—C14	0.6 (6)	C36—C31—P1—C21	−108.4 (3)
C12—C13—C14—C15	0.8 (6)	C32—C31—P1—Mn1	−56.1 (3)
C13—C14—C15—C16	−1.0 (7)	C36—C31—P1—Mn1	124.3 (3)
C12—C11—C16—C15	1.3 (6)	C22—C21—P1—C11	−99.7 (3)
P1—C11—C16—C15	−177.1 (3)	C26—C21—P1—C11	77.1 (3)
C14—C15—C16—C11	0.0 (7)	C22—C21—P1—C31	6.8 (3)
C26—C21—C22—C23	1.4 (6)	C26—C21—P1—C31	−176.4 (3)
P1—C21—C22—C23	178.2 (3)	C22—C21—P1—Mn1	130.3 (3)
C21—C22—C23—C24	−0.9 (6)	C26—C21—P1—Mn1	−52.9 (3)
C22—C23—C24—C25	−0.5 (6)		

Dicarbonyl(η^5-cyclopentadienyl)(tricyclohexylphosphane-κP)manganese(I) (compd2a)

Crystal data

[Mn(C$_5$H$_5$)(C$_{18}$H$_{33}$P)(CO)$_2$]	$F(000) = 976$
$M_r = 456.46$	$D_x = 1.299$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.8938$ (5) Å	Cell parameters from 3157 reflections
$b = 13.6564$ (5) Å	$\theta = 4.5$–28.4°
$c = 17.9372$ (9) Å	$\mu = 0.65$ mm^{-1}
$\beta = 105.676$ (5)°	$T = 173$ K
$V = 2333.42$ (19) Å^3	Block, yellow
$Z = 4$	0.33 × 0.23 × 0.14 mm

Data collection

Oxford Diffraction KM4 Xcalibur2 diffractometer	15861 measured reflections
Radiation source: Enhance (Mo) X-ray Source	5333 independent reflections
Detector resolution: 15.9809 pixels mm^{-1}	3805 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.054$
Absorption correction: multi-scan (CrysAlis PRO; Agilent, 2014)	$\theta_{max} = 27.5°$, $\theta_{min} = 4.3°$
$T_{min} = 0.990$, $T_{max} = 1$	$h = -12 \rightarrow 12$
	$k = -16 \rightarrow 17$
	$l = -23 \rightarrow 18$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 0.4858P]$
$wR(F^2) = 0.119$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.001$
5333 reflections	$\Delta\rho_{max} = 0.67$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.46$ e Å^{-3}
1 restraint	
Primary atom site location: dual	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.7611 (3)	0.38726 (17)	0.34525 (16)	0.0367 (6)
H1	0.764779	0.351126	0.300583	0.044*
C2	0.6679 (3)	0.3703 (2)	0.39079 (18)	0.0469 (8)
H2	0.597698	0.320942	0.382603	0.056*
C3	0.6987 (4)	0.4412 (2)	0.45176 (17)	0.0594 (10)
H3	0.652622	0.447328	0.491615	0.071*
C4	0.8086 (4)	0.4998 (2)	0.44234 (18)	0.0562 (9)
H4	0.849542	0.552989	0.474736	0.067*
C5	0.8485 (3)	0.4672 (2)	0.37718 (18)	0.0434 (7)
H5	0.921073	0.494087	0.357978	0.052*
C6	0.6494 (3)	0.64418 (18)	0.35067 (14)	0.0305 (6)
C7	0.4569 (3)	0.51955 (16)	0.34757 (15)	0.0317 (6)
C11	0.7375 (2)	0.52175 (15)	0.17777 (13)	0.0215 (5)
H11	0.794058	0.466388	0.206906	0.026*
C12	0.7254 (3)	0.50009 (19)	0.09250 (15)	0.0303 (6)
H12A	0.679522	0.555846	0.060163	0.036*
H12B	0.666779	0.441117	0.076037	0.036*
C13	0.8715 (3)	0.48330 (19)	0.08095 (16)	0.0344 (6)
H13A	0.914714	0.425093	0.110970	0.041*
H13B	0.862572	0.470166	0.025551	0.041*
C14	0.9659 (3)	0.57159 (19)	0.10685 (16)	0.0341 (6)

H14A	1.060991	0.556963	0.101666	0.041*
H14B	0.928277	0.628084	0.073025	0.041*
C15	0.9755 (3)	0.5979 (2)	0.19010 (16)	0.0377 (6)
H15A	1.031046	0.658695	0.204132	0.045*
H15B	1.024634	0.544889	0.224589	0.045*
C16	0.8300 (3)	0.61277 (18)	0.20199 (16)	0.0327 (6)
H16A	0.784372	0.669719	0.171102	0.039*
H16B	0.839202	0.627196	0.257228	0.039*
C21	0.4646 (2)	0.42878 (15)	0.15426 (13)	0.0205 (5)
H21	0.450925	0.445970	0.098513	0.025*
C22	0.5318 (2)	0.32681 (16)	0.16678 (15)	0.0286 (5)
H22A	0.626216	0.329503	0.157929	0.034*
H22B	0.542785	0.305990	0.220969	0.034*
C23	0.4416 (3)	0.25222 (17)	0.11176 (16)	0.0343 (6)
H23A	0.435595	0.270886	0.057630	0.041*
H23B	0.486372	0.186926	0.121429	0.041*
C24	0.2948 (3)	0.24676 (17)	0.12253 (16)	0.0337 (6)
H24A	0.299753	0.219288	0.174272	0.040*
H24B	0.236569	0.202344	0.083107	0.040*
C25	0.2266 (3)	0.34721 (18)	0.11517 (17)	0.0373 (6)
H25A	0.135837	0.342255	0.128288	0.045*
H25B	0.207024	0.369568	0.060791	0.045*
C26	0.3192 (2)	0.42289 (16)	0.16810 (16)	0.0302 (6)
H26A	0.273518	0.487923	0.158613	0.036*
H26B	0.328861	0.405077	0.222801	0.036*
C31	0.4871 (2)	0.64279 (15)	0.17097 (13)	0.0207 (5)
H31	0.562728	0.693537	0.181997	0.025*
C32	0.4260 (3)	0.64327 (16)	0.08268 (14)	0.0268 (5)
H32A	0.498317	0.620144	0.057962	0.032*
H32B	0.345683	0.597352	0.068337	0.032*
C33	0.3769 (3)	0.74529 (17)	0.05231 (15)	0.0321 (6)
H33A	0.458502	0.790152	0.062831	0.038*
H33B	0.335690	0.742325	−0.004445	0.038*
C34	0.2687 (3)	0.7848 (2)	0.09036 (17)	0.0398 (7)
H34A	0.182634	0.744313	0.074922	0.048*
H34B	0.243600	0.852664	0.072562	0.048*
C35	0.3257 (3)	0.78358 (19)	0.17777 (16)	0.0394 (7)
H35A	0.251539	0.805962	0.201455	0.047*
H35B	0.405304	0.829902	0.193298	0.047*
C36	0.3750 (2)	0.68134 (16)	0.20837 (14)	0.0263 (5)
H36A	0.293975	0.635974	0.196846	0.032*
H36B	0.414442	0.684082	0.265275	0.032*
O1	0.6626 (2)	0.72846 (13)	0.35804 (11)	0.0437 (5)
O2	0.3426 (2)	0.51997 (13)	0.35504 (13)	0.0448 (5)
P1	0.57562 (6)	0.52605 (4)	0.21266 (3)	0.01882 (14)
Mn1	0.63267 (4)	0.51576 (2)	0.34357 (2)	0.02641 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0460 (16)	0.0260 (12)	0.0338 (15)	0.0114 (12)	0.0036 (12)	0.0026 (11)
C2	0.066 (2)	0.0351 (15)	0.0414 (18)	0.0156 (14)	0.0185 (15)	0.0168 (13)
C3	0.103 (3)	0.0538 (19)	0.0231 (16)	0.0384 (19)	0.0208 (17)	0.0161 (14)
C4	0.076 (2)	0.0472 (17)	0.0297 (17)	0.0177 (17)	−0.0130 (16)	−0.0045 (14)
C5	0.0402 (17)	0.0390 (15)	0.0408 (18)	0.0118 (13)	−0.0065 (13)	−0.0013 (13)
C6	0.0361 (15)	0.0320 (13)	0.0227 (13)	0.0012 (11)	0.0067 (11)	−0.0012 (10)
C7	0.0516 (17)	0.0206 (11)	0.0263 (14)	−0.0013 (11)	0.0163 (12)	−0.0008 (10)
C11	0.0200 (11)	0.0207 (10)	0.0239 (13)	0.0013 (9)	0.0062 (9)	−0.0006 (9)
C12	0.0232 (12)	0.0434 (14)	0.0260 (14)	−0.0061 (11)	0.0099 (10)	−0.0094 (11)
C13	0.0319 (14)	0.0415 (14)	0.0344 (15)	−0.0018 (11)	0.0168 (12)	−0.0112 (12)
C14	0.0242 (13)	0.0422 (15)	0.0382 (16)	−0.0023 (11)	0.0124 (11)	−0.0053 (12)
C15	0.0242 (13)	0.0477 (16)	0.0405 (17)	−0.0096 (12)	0.0078 (11)	−0.0134 (13)
C16	0.0306 (14)	0.0341 (13)	0.0351 (15)	−0.0063 (11)	0.0122 (11)	−0.0130 (11)
C21	0.0243 (12)	0.0185 (10)	0.0193 (12)	−0.0010 (9)	0.0072 (9)	−0.0009 (9)
C22	0.0295 (13)	0.0192 (11)	0.0367 (15)	0.0018 (10)	0.0082 (11)	−0.0040 (10)
C23	0.0439 (16)	0.0223 (11)	0.0377 (16)	−0.0026 (11)	0.0126 (13)	−0.0088 (11)
C24	0.0384 (15)	0.0245 (12)	0.0369 (15)	−0.0092 (11)	0.0081 (12)	−0.0043 (11)
C25	0.0271 (14)	0.0349 (14)	0.0473 (18)	−0.0060 (11)	0.0056 (12)	−0.0003 (12)
C26	0.0267 (13)	0.0228 (11)	0.0436 (16)	−0.0028 (10)	0.0137 (11)	−0.0035 (11)
C31	0.0237 (12)	0.0162 (10)	0.0230 (12)	0.0004 (9)	0.0079 (9)	0.0017 (8)
C32	0.0311 (13)	0.0254 (11)	0.0232 (13)	0.0085 (10)	0.0065 (10)	0.0008 (9)
C33	0.0415 (16)	0.0291 (12)	0.0251 (14)	0.0077 (11)	0.0081 (11)	0.0073 (10)
C34	0.0463 (17)	0.0341 (13)	0.0416 (17)	0.0188 (12)	0.0165 (13)	0.0144 (12)
C35	0.0518 (17)	0.0325 (13)	0.0398 (17)	0.0216 (13)	0.0224 (14)	0.0064 (12)
C36	0.0300 (13)	0.0242 (11)	0.0286 (13)	0.0064 (10)	0.0144 (11)	0.0024 (10)
O1	0.0549 (13)	0.0270 (10)	0.0456 (13)	−0.0067 (9)	0.0075 (10)	−0.0080 (8)
O2	0.0512 (13)	0.0401 (11)	0.0554 (14)	−0.0004 (9)	0.0353 (11)	0.0000 (9)
P1	0.0208 (3)	0.0172 (3)	0.0187 (3)	0.0012 (2)	0.0059 (2)	−0.0011 (2)
Mn1	0.0369 (2)	0.02214 (19)	0.0193 (2)	0.00448 (15)	0.00604 (16)	0.00038 (14)

Geometric parameters (Å, °)

C1—C2	1.407 (4)	C21—C26	1.527 (3)
C1—C5	1.414 (4)	C21—C22	1.533 (3)
C1—Mn1	2.162 (2)	C21—P1	1.856 (2)
C1—H1	0.9500	C21—H21	1.0000
C2—C3	1.431 (4)	C22—C23	1.527 (3)
C2—Mn1	2.151 (3)	C22—H22A	0.9900
C2—H2	0.9500	C22—H22B	0.9900
C3—C4	1.396 (5)	C23—C24	1.517 (4)
C3—Mn1	2.132 (3)	C23—H23A	0.9900
C3—H3	0.9500	C23—H23B	0.9900
C4—C5	1.403 (5)	C24—C25	1.519 (3)
C4—Mn1	2.133 (3)	C24—H24A	0.9900
C4—H4	0.9500	C24—H24B	0.9900

C5—Mn1	2.160 (3)	C25—C26	1.529 (3)
C5—H5	0.9500	C25—H25A	0.9900
C6—O1	1.162 (3)	C25—H25B	0.9900
C6—Mn1	1.763 (3)	C26—H26A	0.9900
C7—O2	1.174 (3)	C26—H26B	0.9900
C7—Mn1	1.761 (3)	C31—C32	1.535 (3)
C11—C12	1.531 (3)	C31—C36	1.535 (3)
C11—C16	1.535 (3)	C31—P1	1.875 (2)
C11—P1	1.871 (2)	C31—H31	1.0000
C11—H11	1.0000	C32—C33	1.527 (3)
C12—C13	1.532 (3)	C32—H32A	0.9900
C12—H12A	0.9900	C32—H32B	0.9900
C12—H12B	0.9900	C33—C34	1.516 (4)
C13—C14	1.519 (3)	C33—H33A	0.9900
C13—H13A	0.9900	C33—H33B	0.9900
C13—H13B	0.9900	C34—C35	1.516 (4)
C14—C15	1.514 (4)	C34—H34A	0.9900
C14—H14A	0.9900	C34—H34B	0.9900
C14—H14B	0.9900	C35—C36	1.531 (3)
C15—C16	1.525 (3)	C35—H35A	0.9900
C15—H15A	0.9900	C35—H35B	0.9900
C15—H15B	0.9900	C36—H36A	0.9900
C16—H16A	0.9900	C36—H36B	0.9900
C16—H16B	0.9900	P1—Mn1	2.2661 (7)
C2—C1—C5	108.5 (3)	C23—C24—H24A	109.4
C2—C1—Mn1	70.55 (15)	C25—C24—H24A	109.4
C5—C1—Mn1	70.82 (15)	C23—C24—H24B	109.4
C2—C1—H1	125.8	C25—C24—H24B	109.4
C5—C1—H1	125.8	H24A—C24—H24B	108.0
Mn1—C1—H1	124.5	C24—C25—C26	112.3 (2)
C1—C2—C3	107.1 (3)	C24—C25—H25A	109.2
C1—C2—Mn1	71.38 (15)	C26—C25—H25A	109.2
C3—C2—Mn1	69.76 (15)	C24—C25—H25B	109.2
C1—C2—H2	126.4	C26—C25—H25B	109.2
C3—C2—H2	126.4	H25A—C25—H25B	107.9
Mn1—C2—H2	124.1	C21—C26—C25	111.5 (2)
C4—C3—C2	107.9 (3)	C21—C26—H26A	109.3
C4—C3—Mn1	70.93 (17)	C25—C26—H26A	109.3
C2—C3—Mn1	71.22 (16)	C21—C26—H26B	109.3
C4—C3—H3	126.0	C25—C26—H26B	109.3
C2—C3—H3	126.0	H26A—C26—H26B	108.0
Mn1—C3—H3	123.5	C32—C31—C36	108.66 (18)
C3—C4—C5	108.8 (3)	C32—C31—P1	115.25 (15)
C3—C4—Mn1	70.86 (18)	C36—C31—P1	115.59 (15)
C5—C4—Mn1	71.98 (16)	C32—C31—H31	105.4
C3—C4—H4	125.6	C36—C31—H31	105.4
C5—C4—H4	125.6	P1—C31—H31	105.4

Mn1—C4—H4	123.2	C33—C32—C31	111.76 (19)
C4—C5—C1	107.6 (3)	C33—C32—H32A	109.3
C4—C5—Mn1	69.87 (18)	C31—C32—H32A	109.3
C1—C5—Mn1	70.98 (15)	C33—C32—H32B	109.3
C4—C5—H5	126.2	C31—C32—H32B	109.3
C1—C5—H5	126.2	H32A—C32—H32B	107.9
Mn1—C5—H5	124.6	C34—C33—C32	111.1 (2)
O1—C6—Mn1	177.7 (2)	C34—C33—H33A	109.4
O2—C7—Mn1	175.7 (2)	C32—C33—H33A	109.4
C12—C11—C16	108.59 (19)	C34—C33—H33B	109.4
C12—C11—P1	119.85 (16)	C32—C33—H33B	109.4
C16—C11—P1	112.24 (15)	H33A—C33—H33B	108.0
C12—C11—H11	104.9	C33—C34—C35	110.6 (2)
C16—C11—H11	104.9	C33—C34—H34A	109.5
P1—C11—H11	104.9	C35—C34—H34A	109.5
C11—C12—C13	110.0 (2)	C33—C34—H34B	109.5
C11—C12—H12A	109.7	C35—C34—H34B	109.5
C13—C12—H12A	109.7	H34A—C34—H34B	108.1
C11—C12—H12B	109.7	C34—C35—C36	112.0 (2)
C13—C12—H12B	109.7	C34—C35—H35A	109.2
H12A—C12—H12B	108.2	C36—C35—H35A	109.2
C14—C13—C12	111.4 (2)	C34—C35—H35B	109.2
C14—C13—H13A	109.4	C36—C35—H35B	109.2
C12—C13—H13A	109.4	H35A—C35—H35B	107.9
C14—C13—H13B	109.4	C35—C36—C31	110.73 (19)
C12—C13—H13B	109.4	C35—C36—H36A	109.5
H13A—C13—H13B	108.0	C31—C36—H36A	109.5
C15—C14—C13	111.1 (2)	C35—C36—H36B	109.5
C15—C14—H14A	109.4	C31—C36—H36B	109.5
C13—C14—H14A	109.4	H36A—C36—H36B	108.1
C15—C14—H14B	109.4	C21—P1—C11	102.59 (10)
C13—C14—H14B	109.4	C21—P1—C31	104.00 (10)
H14A—C14—H14B	108.0	C11—P1—C31	104.08 (10)
C14—C15—C16	111.1 (2)	C21—P1—Mn1	118.96 (7)
C14—C15—H15A	109.4	C11—P1—Mn1	110.40 (8)
C16—C15—H15A	109.4	C31—P1—Mn1	115.14 (7)
C14—C15—H15B	109.4	C7—Mn1—C6	92.44 (11)
C16—C15—H15B	109.4	C7—Mn1—C3	92.30 (14)
H15A—C15—H15B	108.0	C6—Mn1—C3	114.18 (12)
C15—C16—C11	111.44 (19)	C7—Mn1—C4	124.22 (14)
C15—C16—H16A	109.3	C6—Mn1—C4	90.11 (12)
C11—C16—H16A	109.3	C3—Mn1—C4	38.21 (14)
C15—C16—H16B	109.3	C7—Mn1—C2	93.89 (12)
C11—C16—H16B	109.3	C6—Mn1—C2	152.66 (12)
H16A—C16—H16B	108.0	C3—Mn1—C2	39.03 (12)
C26—C21—C22	108.56 (18)	C4—Mn1—C2	64.49 (13)
C26—C21—P1	112.69 (15)	C7—Mn1—C5	155.56 (12)
C22—C21—P1	113.60 (15)	C6—Mn1—C5	102.61 (11)

C26—C21—H21	107.2	C3—Mn1—C5	64.06 (13)
C22—C21—H21	107.2	C4—Mn1—C5	38.15 (12)
P1—C21—H21	107.2	C2—Mn1—C5	64.15 (12)
C23—C22—C21	110.90 (19)	C7—Mn1—C1	127.35 (11)
C23—C22—H22A	109.5	C6—Mn1—C1	139.72 (11)
C21—C22—H22A	109.5	C3—Mn1—C1	64.22 (11)
C23—C22—H22B	109.5	C4—Mn1—C1	63.95 (11)
C21—C22—H22B	109.5	C2—Mn1—C1	38.06 (11)
H22A—C22—H22B	108.0	C5—Mn1—C1	38.20 (10)
C24—C23—C22	111.3 (2)	C7—Mn1—P1	93.91 (9)
C24—C23—H23A	109.4	C6—Mn1—P1	90.31 (8)
C22—C23—H23A	109.4	C3—Mn1—P1	154.43 (9)
C24—C23—H23B	109.4	C4—Mn1—P1	141.81 (11)
C22—C23—H23B	109.4	C2—Mn1—P1	115.70 (9)
H23A—C23—H23B	108.0	C5—Mn1—P1	105.01 (9)
C23—C24—C25	111.3 (2)	C1—Mn1—P1	92.62 (8)
C5—C1—C2—C3	0.0 (3)	P1—C21—C26—C25	175.99 (17)
Mn1—C1—C2—C3	−60.94 (18)	C24—C25—C26—C21	55.0 (3)
C5—C1—C2—Mn1	60.96 (18)	C36—C31—C32—C33	57.5 (3)
C1—C2—C3—C4	0.2 (3)	P1—C31—C32—C33	−170.96 (16)
Mn1—C2—C3—C4	−61.8 (2)	C31—C32—C33—C34	−57.4 (3)
C1—C2—C3—Mn1	61.99 (19)	C32—C33—C34—C35	55.2 (3)
C2—C3—C4—C5	−0.4 (3)	C33—C34—C35—C36	−55.6 (3)
Mn1—C3—C4—C5	−62.3 (2)	C34—C35—C36—C31	57.2 (3)
C2—C3—C4—Mn1	62.0 (2)	C32—C31—C36—C35	−56.8 (3)
C3—C4—C5—C1	0.4 (3)	P1—C31—C36—C35	171.86 (18)
Mn1—C4—C5—C1	−61.26 (18)	C26—C21—P1—C11	−175.69 (16)
C3—C4—C5—Mn1	61.6 (2)	C22—C21—P1—C11	60.32 (18)
C2—C1—C5—C4	−0.2 (3)	C26—C21—P1—C31	−67.48 (18)
Mn1—C1—C5—C4	60.55 (19)	C22—C21—P1—C31	168.53 (16)
C2—C1—C5—Mn1	−60.79 (19)	C26—C21—P1—Mn1	62.19 (18)
C16—C11—C12—C13	58.8 (3)	C22—C21—P1—Mn1	−61.81 (18)
P1—C11—C12—C13	−170.43 (16)	C12—C11—P1—C21	36.0 (2)
C11—C12—C13—C14	−58.3 (3)	C16—C11—P1—C21	165.13 (17)
C12—C13—C14—C15	55.7 (3)	C12—C11—P1—C31	−72.20 (19)
C13—C14—C15—C16	−54.4 (3)	C16—C11—P1—C31	56.99 (19)
C14—C15—C16—C11	56.7 (3)	C12—C11—P1—Mn1	163.71 (16)
C12—C11—C16—C15	−58.5 (3)	C16—C11—P1—Mn1	−67.11 (18)
P1—C11—C16—C15	166.64 (18)	C32—C31—P1—C21	−38.13 (19)
C26—C21—C22—C23	59.1 (3)	C36—C31—P1—C21	90.05 (18)
P1—C21—C22—C23	−174.73 (17)	C32—C31—P1—C11	68.97 (18)
C21—C22—C23—C24	−58.3 (3)	C36—C31—P1—C11	−162.85 (17)
C22—C23—C24—C25	54.1 (3)	C32—C31—P1—Mn1	−170.06 (14)
C23—C24—C25—C26	−52.5 (3)	C36—C31—P1—Mn1	−41.88 (19)
C22—C21—C26—C25	−57.3 (3)		

Dicarbonyl(η^5-1-chlorocyclopentadienyl)(tricyclohexylphosphane-κP)manganese(I) (compd2b)

Crystal data

[Mn(C$_5$H$_4$Cl)(C$_{18}$H$_{33}$P)(CO)$_2$]	$F(000) = 1040$
$M_r = 490.90$	$D_x = 1.387$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 9.6649$ (3) Å	Cell parameters from 9847 reflections
$b = 13.9301$ (4) Å	$\theta = 2.7–26.4°$
$c = 17.9790$ (6) Å	$\mu = 0.76$ mm^{-1}
$\beta = 103.835$ (1)°	$T = 100$ K
$V = 2350.34$ (13) Å^3	Block, brown
$Z = 4$	$0.10 \times 0.08 \times 0.06$ mm

Data collection

Bruker D8 Venture diffractometer	31339 measured reflections
Radiation source: rotating anode generator, Bruker TXS	4809 independent reflections
	4098 reflections with $I > 2\sigma(I)$
Detector resolution: 7.4074 pixels mm^{-1}	$R_{int} = 0.039$
mix of ω and phi scans	$\theta_{max} = 26.4°$, $\theta_{min} = 2.8°$
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)	$h = -12\rightarrow12$
	$k = -17\rightarrow17$
$T_{min} = 0.704$, $T_{max} = 0.745$	$l = -22\rightarrow22$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 8.9831P]$
$wR(F^2) = 0.149$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
4809 reflections	$\Delta\rho_{max} = 0.73$ e Å^{-3}
271 parameters	$\Delta\rho_{min} = -1.63$ e Å^{-3}
1 restraint	
Primary atom site location: dual	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4427 (4)	0.4285 (3)	0.1227 (2)	0.0347 (10)
C2	0.5217 (5)	0.4090 (3)	0.0659 (2)	0.0397 (9)
H2	0.496315	0.363858	0.025362	0.048*
C3	0.6412 (5)	0.4675 (3)	0.0807 (2)	0.0382 (8)
H3	0.711760	0.469712	0.051846	0.046*
C4	0.6397 (4)	0.5235 (3)	0.1462 (2)	0.0281 (8)
H4	0.708904	0.569982	0.168819	0.034*
C5	0.5169 (4)	0.4983 (2)	0.17256 (19)	0.0203 (7)
H5	0.490198	0.524116	0.216014	0.024*

C6	0.6116 (3)	0.2484 (3)	0.16310 (19)	0.0204 (7)
C7	0.8340 (4)	0.3572 (2)	0.17413 (17)	0.0180 (7)
C11	0.5323 (3)	0.3609 (2)	0.34076 (18)	0.0146 (6)
H11	0.484002	0.422568	0.321198	0.017*
C12	0.4269 (3)	0.2816 (2)	0.3053 (2)	0.0221 (7)
H12A	0.415554	0.280687	0.249112	0.026*
H12B	0.465064	0.218481	0.325855	0.026*
C13	0.2816 (3)	0.2981 (3)	0.3232 (2)	0.0242 (7)
H13A	0.239281	0.358041	0.298158	0.029*
H13B	0.217097	0.244380	0.302091	0.029*
C14	0.2946 (4)	0.3053 (3)	0.4090 (2)	0.0266 (8)
H14A	0.324682	0.242394	0.433090	0.032*
H14B	0.200369	0.321133	0.418292	0.032*
C15	0.4022 (4)	0.3818 (3)	0.4457 (2)	0.0264 (8)
H15A	0.413057	0.381436	0.501883	0.032*
H15B	0.366748	0.445849	0.426138	0.032*
C16	0.5475 (3)	0.3631 (3)	0.42776 (19)	0.0208 (7)
H16A	0.615242	0.414225	0.450946	0.025*
H16B	0.585977	0.300918	0.450305	0.025*
C21	0.8095 (3)	0.4529 (2)	0.36170 (17)	0.0133 (6)
H21	0.831092	0.432593	0.416620	0.016*
C22	0.7340 (4)	0.5510 (2)	0.3559 (2)	0.0188 (7)
H22A	0.708557	0.572188	0.301780	0.023*
H22B	0.644921	0.544678	0.373500	0.023*
C23	0.8299 (4)	0.6264 (2)	0.4046 (2)	0.0220 (7)
H23A	0.849513	0.607659	0.459257	0.026*
H23B	0.780200	0.689086	0.398842	0.026*
C24	0.9707 (4)	0.6363 (2)	0.3805 (2)	0.0224 (7)
H24A	0.951748	0.660552	0.327261	0.027*
H24B	1.032396	0.683468	0.414155	0.027*
C25	1.0473 (4)	0.5402 (2)	0.38564 (19)	0.0201 (7)
H25A	1.076387	0.519824	0.439897	0.024*
H25B	1.134476	0.547445	0.366367	0.024*
C26	0.9518 (3)	0.4633 (2)	0.33897 (18)	0.0159 (6)
H26A	1.002458	0.400916	0.346422	0.019*
H26B	0.933107	0.479851	0.283920	0.019*
C31	0.7847 (3)	0.2428 (2)	0.34542 (17)	0.0126 (6)
H31	0.705552	0.195282	0.340811	0.015*
C32	0.8604 (3)	0.2453 (2)	0.43095 (18)	0.0164 (6)
H32A	0.946698	0.285918	0.438502	0.020*
H32B	0.796260	0.273997	0.460322	0.020*
C33	0.9028 (4)	0.1436 (2)	0.46096 (19)	0.0200 (7)
H33A	0.951208	0.146833	0.516053	0.024*
H33B	0.816029	0.103915	0.455618	0.024*
C34	1.0016 (4)	0.0967 (2)	0.41725 (19)	0.0217 (7)
H34A	1.020950	0.029548	0.434804	0.026*
H34B	1.093484	0.131567	0.427779	0.026*
C35	0.9343 (4)	0.0978 (2)	0.33147 (19)	0.0209 (7)

H35A	0.850244	0.054864	0.320488	0.025*
H35B	1.003714	0.072387	0.303879	0.025*
C36	0.8882 (3)	0.1984 (2)	0.30160 (18)	0.0159 (6)
H36A	0.841022	0.194922	0.246354	0.019*
H36B	0.973263	0.239976	0.307612	0.019*
Cl1	0.27801 (13)	0.38736 (9)	0.11798 (9)	0.0547 (4)
O1	0.5821 (3)	0.16805 (19)	0.15191 (16)	0.0316 (6)
O2	0.9512 (3)	0.35257 (17)	0.16860 (14)	0.0212 (5)
P1	0.69764 (8)	0.35770 (5)	0.30450 (4)	0.01128 (18)
Mn1	0.65220 (5)	0.37253 (3)	0.17494 (3)	0.01568 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0245 (19)	0.0275 (19)	0.040 (2)	0.0105 (15)	−0.0170 (16)	−0.0051 (17)
C2	0.057 (2)	0.034 (2)	0.0168 (17)	0.0264 (14)	−0.0120 (17)	−0.0049 (16)
C3	0.058 (2)	0.038 (2)	0.0208 (18)	0.0255 (14)	0.0121 (17)	0.0155 (16)
C4	0.037 (2)	0.0183 (17)	0.0291 (19)	0.0112 (15)	0.0082 (16)	0.0112 (15)
C5	0.0205 (16)	0.0167 (15)	0.0205 (16)	0.0073 (13)	−0.0012 (13)	0.0000 (13)
C6	0.0134 (14)	0.0270 (18)	0.0186 (16)	0.0023 (13)	−0.0002 (12)	−0.0020 (13)
C7	0.0343 (19)	0.0100 (14)	0.0086 (14)	0.0008 (13)	0.0032 (13)	0.0005 (11)
C11	0.0105 (13)	0.0137 (14)	0.0198 (15)	−0.0001 (11)	0.0040 (12)	−0.0004 (12)
C12	0.0129 (15)	0.0221 (16)	0.0317 (18)	−0.0018 (13)	0.0064 (13)	−0.0060 (14)
C13	0.0111 (15)	0.0299 (18)	0.0317 (19)	−0.0010 (13)	0.0054 (13)	−0.0031 (15)
C14	0.0137 (15)	0.035 (2)	0.0327 (19)	0.0010 (14)	0.0083 (14)	0.0069 (16)
C15	0.0183 (16)	0.041 (2)	0.0218 (17)	0.0023 (15)	0.0091 (14)	−0.0005 (15)
C16	0.0130 (15)	0.0315 (18)	0.0192 (16)	−0.0019 (13)	0.0061 (12)	0.0003 (14)
C21	0.0143 (14)	0.0131 (14)	0.0128 (14)	0.0004 (11)	0.0038 (11)	0.0002 (11)
C22	0.0199 (16)	0.0125 (14)	0.0241 (16)	0.0027 (12)	0.0053 (13)	−0.0019 (12)
C23	0.0285 (18)	0.0133 (15)	0.0240 (17)	−0.0004 (13)	0.0060 (14)	−0.0023 (13)
C24	0.0304 (18)	0.0175 (16)	0.0178 (16)	−0.0084 (14)	0.0031 (14)	−0.0008 (13)
C25	0.0201 (16)	0.0209 (16)	0.0178 (15)	−0.0051 (13)	0.0014 (13)	−0.0003 (13)
C26	0.0160 (15)	0.0149 (14)	0.0169 (15)	−0.0027 (12)	0.0045 (12)	−0.0019 (12)
C31	0.0135 (14)	0.0116 (13)	0.0131 (14)	0.0001 (11)	0.0038 (11)	0.0007 (11)
C32	0.0183 (15)	0.0167 (15)	0.0140 (14)	0.0029 (12)	0.0037 (12)	−0.0008 (12)
C33	0.0258 (17)	0.0193 (16)	0.0159 (15)	0.0048 (13)	0.0073 (13)	0.0046 (12)
C34	0.0266 (17)	0.0173 (15)	0.0216 (16)	0.0085 (13)	0.0069 (14)	0.0074 (13)
C35	0.0292 (18)	0.0164 (15)	0.0187 (16)	0.0073 (13)	0.0090 (14)	0.0015 (13)
C36	0.0188 (15)	0.0155 (14)	0.0148 (14)	0.0034 (12)	0.0071 (12)	0.0017 (12)
Cl1	0.0345 (6)	0.0374 (6)	0.0816 (9)	−0.0003 (5)	−0.0068 (6)	0.0004 (6)
O1	0.0318 (14)	0.0226 (13)	0.0388 (16)	−0.0093 (11)	0.0054 (12)	−0.0096 (12)
O2	0.0237 (13)	0.0207 (12)	0.0224 (12)	−0.0003 (9)	0.0122 (10)	−0.0002 (9)
P1	0.0105 (4)	0.0113 (4)	0.0119 (4)	0.0012 (3)	0.0025 (3)	−0.0002 (3)
Mn1	0.0188 (3)	0.0151 (3)	0.0113 (2)	0.00472 (18)	−0.00016 (18)	−0.00018 (17)

Geometric parameters (Å, º)

C1—C5	1.399 (5)	C21—C26	1.533 (4)
C1—C2	1.439 (6)	C21—C22	1.541 (4)
C1—Cl1	1.674 (4)	C21—P1	1.858 (3)
C1—Mn1	2.164 (4)	C21—H21	1.0000
C2—C3	1.387 (7)	C22—C23	1.530 (5)
C2—Mn1	2.123 (4)	C22—H22A	0.9900
C2—H2	0.9500	C22—H22B	0.9900
C3—C4	1.416 (6)	C23—C24	1.530 (5)
C3—Mn1	2.133 (4)	C23—H23A	0.9900
C3—H3	0.9500	C23—H23B	0.9900
C4—C5	1.423 (5)	C24—C25	1.522 (5)
C4—Mn1	2.162 (4)	C24—H24A	0.9900
C4—H4	0.9500	C24—H24B	0.9900
C5—Mn1	2.180 (3)	C25—C26	1.528 (4)
C5—H5	0.9500	C25—H25A	0.9900
C6—O1	1.160 (4)	C25—H25B	0.9900
C6—Mn1	1.775 (4)	C26—H26A	0.9900
C7—O2	1.162 (4)	C26—H26B	0.9900
C7—Mn1	1.774 (4)	C31—C32	1.537 (4)
C11—C12	1.535 (4)	C31—C36	1.542 (4)
C11—C16	1.536 (4)	C31—P1	1.875 (3)
C11—P1	1.865 (3)	C31—H31	1.0000
C11—H11	1.0000	C32—C33	1.536 (4)
C12—C13	1.531 (4)	C32—H32A	0.9900
C12—H12A	0.9900	C32—H32B	0.9900
C12—H12B	0.9900	C33—C34	1.522 (5)
C13—C14	1.519 (5)	C33—H33A	0.9900
C13—H13A	0.9900	C33—H33B	0.9900
C13—H13B	0.9900	C34—C35	1.524 (5)
C14—C15	1.524 (5)	C34—H34A	0.9900
C14—H14A	0.9900	C34—H34B	0.9900
C14—H14B	0.9900	C35—C36	1.529 (4)
C15—C16	1.537 (4)	C35—H35A	0.9900
C15—H15A	0.9900	C35—H35B	0.9900
C15—H15B	0.9900	C36—H36A	0.9900
C16—H16A	0.9900	C36—H36B	0.9900
C16—H16B	0.9900	P1—Mn1	2.2743 (9)
C5—C1—C2	107.9 (4)	C25—C24—H24A	109.5
C5—C1—Cl1	127.3 (3)	C23—C24—H24A	109.5
C2—C1—Cl1	124.0 (3)	C25—C24—H24B	109.5
C5—C1—Mn1	71.9 (2)	C23—C24—H24B	109.5
C2—C1—Mn1	68.9 (2)	H24A—C24—H24B	108.1
Cl1—C1—Mn1	132.7 (2)	C24—C25—C26	111.3 (3)
C3—C2—C1	108.3 (3)	C24—C25—H25A	109.4
C3—C2—Mn1	71.4 (2)	C26—C25—H25A	109.4

C1—C2—Mn1	71.9 (2)	C24—C25—H25B	109.4
C3—C2—H2	125.9	C26—C25—H25B	109.4
C1—C2—H2	125.9	H25A—C25—H25B	108.0
Mn1—C2—H2	122.5	C25—C26—C21	112.5 (3)
C2—C3—C4	107.9 (4)	C25—C26—H26A	109.1
C2—C3—Mn1	70.6 (2)	C21—C26—H26A	109.1
C4—C3—Mn1	71.8 (2)	C25—C26—H26B	109.1
C2—C3—H3	126.0	C21—C26—H26B	109.1
C4—C3—H3	126.0	H26A—C26—H26B	107.8
Mn1—C3—H3	123.2	C32—C31—C36	108.0 (2)
C3—C4—C5	108.5 (4)	C32—C31—P1	115.8 (2)
C3—C4—Mn1	69.7 (2)	C36—C31—P1	115.3 (2)
C5—C4—Mn1	71.6 (2)	C32—C31—H31	105.6
C3—C4—H4	125.8	C36—C31—H31	105.6
C5—C4—H4	125.8	P1—C31—H31	105.6
Mn1—C4—H4	124.6	C33—C32—C31	110.7 (3)
C1—C5—C4	107.4 (3)	C33—C32—H32A	109.5
C1—C5—Mn1	70.6 (2)	C31—C32—H32A	109.5
C4—C5—Mn1	70.15 (19)	C33—C32—H32B	109.5
C1—C5—H5	126.3	C31—C32—H32B	109.5
C4—C5—H5	126.3	H32A—C32—H32B	108.1
Mn1—C5—H5	124.6	C34—C33—C32	111.3 (3)
O1—C6—Mn1	176.9 (3)	C34—C33—H33A	109.4
O2—C7—Mn1	174.3 (3)	C32—C33—H33A	109.4
C12—C11—C16	109.2 (3)	C34—C33—H33B	109.4
C12—C11—P1	112.1 (2)	C32—C33—H33B	109.4
C16—C11—P1	118.4 (2)	H33A—C33—H33B	108.0
C12—C11—H11	105.3	C33—C34—C35	110.5 (3)
C16—C11—H11	105.3	C33—C34—H34A	109.6
P1—C11—H11	105.3	C35—C34—H34A	109.6
C13—C12—C11	110.8 (3)	C33—C34—H34B	109.6
C13—C12—H12A	109.5	C35—C34—H34B	109.6
C11—C12—H12A	109.5	H34A—C34—H34B	108.1
C13—C12—H12B	109.5	C34—C35—C36	112.5 (3)
C11—C12—H12B	109.5	C34—C35—H35A	109.1
H12A—C12—H12B	108.1	C36—C35—H35A	109.1
C14—C13—C12	111.5 (3)	C34—C35—H35B	109.1
C14—C13—H13A	109.3	C36—C35—H35B	109.1
C12—C13—H13A	109.3	H35A—C35—H35B	107.8
C14—C13—H13B	109.3	C35—C36—C31	111.0 (2)
C12—C13—H13B	109.3	C35—C36—H36A	109.4
H13A—C13—H13B	108.0	C31—C36—H36A	109.4
C13—C14—C15	111.6 (3)	C35—C36—H36B	109.4
C13—C14—H14A	109.3	C31—C36—H36B	109.4
C15—C14—H14A	109.3	H36A—C36—H36B	108.0
C13—C14—H14B	109.3	C21—P1—C11	102.88 (14)
C15—C14—H14B	109.3	C21—P1—C31	104.18 (13)
H14A—C14—H14B	108.0	C11—P1—C31	103.02 (14)

C14—C15—C16	110.7 (3)	C21—P1—Mn1	116.51 (10)
C14—C15—H15A	109.5	C11—P1—Mn1	112.59 (10)
C16—C15—H15A	109.5	C31—P1—Mn1	115.98 (10)
C14—C15—H15B	109.5	C7—Mn1—C6	94.18 (14)
C16—C15—H15B	109.5	C7—Mn1—C2	113.10 (17)
H15A—C15—H15B	108.1	C6—Mn1—C2	93.27 (16)
C11—C16—C15	110.3 (3)	C7—Mn1—C3	85.94 (16)
C11—C16—H16A	109.6	C6—Mn1—C3	122.80 (17)
C15—C16—H16A	109.6	C2—Mn1—C3	38.04 (19)
C11—C16—H16B	109.6	C7—Mn1—C4	96.56 (15)
C15—C16—H16B	109.6	C6—Mn1—C4	157.08 (15)
H16A—C16—H16B	108.1	C2—Mn1—C4	63.88 (16)
C26—C21—C22	109.8 (2)	C3—Mn1—C4	38.50 (15)
C26—C21—P1	111.1 (2)	C7—Mn1—C1	150.01 (16)
C22—C21—P1	113.1 (2)	C6—Mn1—C1	98.13 (15)
C26—C21—H21	107.5	C2—Mn1—C1	39.20 (17)
C22—C21—H21	107.5	C3—Mn1—C1	64.41 (18)
P1—C21—H21	107.5	C4—Mn1—C1	63.44 (16)
C23—C22—C21	111.0 (3)	C7—Mn1—C5	133.42 (14)
C23—C22—H22A	109.4	C6—Mn1—C5	131.76 (14)
C21—C22—H22A	109.4	C2—Mn1—C5	64.43 (14)
C23—C22—H22B	109.4	C3—Mn1—C5	64.56 (14)
C21—C22—H22B	109.4	C4—Mn1—C5	38.25 (14)
H22A—C22—H22B	108.0	C1—Mn1—C5	37.58 (14)
C22—C23—C24	111.0 (3)	C7—Mn1—P1	92.77 (10)
C22—C23—H23A	109.4	C6—Mn1—P1	90.99 (11)
C24—C23—H23A	109.4	C2—Mn1—P1	153.34 (13)
C22—C23—H23B	109.4	C3—Mn1—P1	146.20 (13)
C24—C23—H23B	109.4	C4—Mn1—P1	108.60 (11)
H23A—C23—H23B	108.0	C1—Mn1—P1	114.14 (13)
C25—C24—C23	110.9 (3)	C5—Mn1—P1	93.50 (9)
C5—C1—C2—C3	−0.9 (4)	C23—C24—C25—C26	55.1 (4)
Cl1—C1—C2—C3	169.4 (3)	C24—C25—C26—C21	−55.0 (4)
Mn1—C1—C2—C3	−62.5 (3)	C22—C21—C26—C25	54.8 (3)
C5—C1—C2—Mn1	61.6 (3)	P1—C21—C26—C25	−179.3 (2)
Cl1—C1—C2—Mn1	−128.1 (3)	C36—C31—C32—C33	−59.6 (3)
C1—C2—C3—C4	0.3 (4)	P1—C31—C32—C33	169.5 (2)
Mn1—C2—C3—C4	−62.5 (3)	C31—C32—C33—C34	59.1 (4)
C1—C2—C3—Mn1	62.9 (3)	C32—C33—C34—C35	−54.6 (4)
C2—C3—C4—C5	0.4 (4)	C33—C34—C35—C36	53.7 (4)
Mn1—C3—C4—C5	−61.4 (2)	C34—C35—C36—C31	−56.3 (4)
C2—C3—C4—Mn1	61.7 (3)	C32—C31—C36—C35	58.0 (3)
C2—C1—C5—C4	1.1 (4)	P1—C31—C36—C35	−170.8 (2)
Cl1—C1—C5—C4	−168.8 (3)	C26—C21—P1—C11	−178.9 (2)
Mn1—C1—C5—C4	60.8 (2)	C22—C21—P1—C11	−54.8 (2)
C2—C1—C5—Mn1	−59.7 (2)	C26—C21—P1—C31	73.9 (2)
Cl1—C1—C5—Mn1	130.4 (4)	C22—C21—P1—C31	−162.1 (2)

C3—C4—C5—C1	−0.9 (4)	C26—C21—P1—Mn1	−55.2 (2)
Mn1—C4—C5—C1	−61.1 (2)	C22—C21—P1—Mn1	68.8 (2)
C3—C4—C5—Mn1	60.2 (2)	C12—C11—P1—C21	−175.6 (2)
C16—C11—C12—C13	58.2 (4)	C16—C11—P1—C21	−47.0 (3)
P1—C11—C12—C13	−168.6 (2)	C12—C11—P1—C31	−67.5 (3)
C11—C12—C13—C14	−56.1 (4)	C16—C11—P1—C31	61.1 (3)
C12—C13—C14—C15	54.5 (4)	C12—C11—P1—Mn1	58.2 (2)
C13—C14—C15—C16	−55.2 (4)	C16—C11—P1—Mn1	−173.3 (2)
C12—C11—C16—C15	−59.1 (4)	C32—C31—P1—C21	30.7 (2)
P1—C11—C16—C15	171.0 (2)	C36—C31—P1—C21	−96.7 (2)
C14—C15—C16—C11	57.8 (4)	C32—C31—P1—C11	−76.4 (2)
C26—C21—C22—C23	−55.9 (3)	C36—C31—P1—C11	156.2 (2)
P1—C21—C22—C23	179.4 (2)	C32—C31—P1—Mn1	160.11 (19)
C21—C22—C23—C24	57.6 (4)	C36—C31—P1—Mn1	32.8 (2)
C22—C23—C24—C25	−56.8 (4)		

Carbonyl*η*^{5}-cyclopentadienyl)[1,2-bis(diphenylphosphanyl)ethane-*κ*^{2}*P*,*P′*]manganese(I) (compd3a)

Crystal data

[Mn(C$_5$H$_5$)(C$_{26}$H$_{24}$P$_2$)(CO)]
M_r = 546.43
Monoclinic, $C2/c$
a = 29.0323 (7) Å
b = 8.9592 (2) Å
c = 26.4794 (7) Å
$β$ = 122.159 (1)°
V = 5830.7 (3) Å^3
Z = 8

$F(000)$ = 2272
D_x = 1.245 Mg m^{-3}
Mo $Kα$ radiation, $λ$ = 0.71073 Å
Cell parameters from 9574 reflections
$θ$ = 2.4–27.5°
$μ$ = 0.58 mm^{-1}
T = 100 K
Block, yellow
0.10 × 0.08 × 0.07 mm

Data collection

Bruker D8 Venture
  diffractometer
Radiation source: rotating anode generator
Detector resolution: 7.4074 pixels mm^{-1}
mix of $ω$ and phi scans
Absorption correction: multi-scan
  (SADABS; Krause *et al.*, 2015)
T_{min} = 0.719, T_{max} = 0.746

70409 measured reflections
6696 independent reflections
6042 reflections with $I > 2σ(I)$
R_{int} = 0.032
$θ_{max}$ = 27.5°, $θ_{min}$ = 3.0°
h = −37→37
k = −11→11
l = −34→34

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2σ(F^2)]$ = 0.030
$wR(F^2)$ = 0.081
S = 1.09
6696 reflections
325 parameters
0 restraints
Primary atom site location: dual

Hydrogen site location: inferred from
  neighbouring sites
H-atom parameters constrained
$w = 1/[σ^2(F_o^2) + (0.0346P)^2 + 9.225P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(Δ/σ)_{max}$ = 0.001
$Δρ_{max}$ = 0.39 e Å^{-3}
$Δρ_{min}$ = −0.36 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.33814 (2)	0.43019 (2)	0.47115 (2)	0.01230 (7)
P1	0.31992 (2)	0.63118 (4)	0.41610 (2)	0.01282 (8)
P2	0.36355 (2)	0.58721 (4)	0.54455 (2)	0.01255 (8)
O1	0.22802 (4)	0.43657 (13)	0.44923 (5)	0.0237 (3)
C131	0.34379 (6)	0.55223 (17)	0.59883 (6)	0.0157 (3)
C116	0.39068 (6)	0.87185 (18)	0.43335 (7)	0.0205 (3)
H116	0.372406	0.925459	0.448582	0.025*
C115	0.43362 (7)	0.93913 (19)	0.43299 (8)	0.0264 (4)
H115	0.444867	1.036968	0.448631	0.032*
C101	0.26537 (6)	0.62584 (17)	0.33645 (6)	0.0150 (3)
C6	0.27215 (6)	0.43543 (16)	0.45789 (7)	0.0164 (3)
C111	0.37384 (6)	0.72736 (17)	0.41184 (7)	0.0165 (3)
C132	0.34854 (6)	0.66310 (18)	0.63857 (7)	0.0179 (3)
H132	0.360325	0.760285	0.636163	0.021*
C133	0.33622 (6)	0.63251 (19)	0.68146 (7)	0.0207 (3)
H133	0.338895	0.709174	0.707678	0.025*
C11	0.29693 (6)	0.77466 (17)	0.44812 (6)	0.0161 (3)
H11A	0.295744	0.873460	0.430721	0.019*
H11B	0.259859	0.750439	0.438606	0.019*
C106	0.26321 (6)	0.72580 (19)	0.29503 (7)	0.0205 (3)
H106	0.290299	0.800875	0.307722	0.025*
C136	0.32685 (7)	0.41047 (18)	0.60331 (7)	0.0217 (3)
H136	0.323065	0.334171	0.576433	0.026*
C4	0.33120 (6)	0.21596 (17)	0.43179 (7)	0.0192 (3)
H4	0.298331	0.175488	0.399613	0.023*
C5	0.36891 (6)	0.30449 (17)	0.42689 (7)	0.0180 (3)
H5	0.365697	0.333869	0.390674	0.022*
C1	0.41258 (6)	0.34233 (18)	0.48540 (7)	0.0196 (3)
H1	0.443483	0.401152	0.495181	0.023*
C12	0.33665 (6)	0.77923 (16)	0.51613 (6)	0.0160 (3)
H12A	0.317689	0.817382	0.535423	0.019*
H12B	0.367184	0.847521	0.526176	0.019*
C104	0.18145 (7)	0.60869 (19)	0.21602 (7)	0.0220 (3)
H104	0.153122	0.602775	0.175161	0.026*
C134	0.32004 (7)	0.4905 (2)	0.68612 (7)	0.0251 (3)
H134	0.312167	0.469006	0.715886	0.030*
C3	0.35132 (7)	0.19821 (17)	0.49375 (7)	0.0213 (3)
H3	0.334185	0.143948	0.510156	0.026*
C105	0.22156 (7)	0.7168 (2)	0.23495 (7)	0.0245 (3)

H105	0.220707	0.784887	0.206970	0.029*
C103	0.18285 (7)	0.50961 (19)	0.25684 (7)	0.0244 (3)
H103	0.155257	0.436050	0.244131	0.029*
C2	0.40130 (7)	0.27578 (18)	0.52636 (7)	0.0218 (3)
H2	0.423600	0.282269	0.568594	0.026*
C122	0.46660 (6)	0.68578 (19)	0.57420 (7)	0.0217 (3)
H122	0.447981	0.720293	0.534147	0.026*
C121	0.43722 (6)	0.61715 (17)	0.59556 (6)	0.0153 (3)
C123	0.52249 (6)	0.70481 (19)	0.61022 (8)	0.0248 (3)
H123	0.541667	0.753723	0.595021	0.030*
C112	0.40068 (7)	0.6535 (2)	0.38845 (9)	0.0276 (4)
H112	0.389731	0.555439	0.372973	0.033*
C102	0.22478 (6)	0.51768 (18)	0.31665 (7)	0.0216 (3)
H102	0.225713	0.448431	0.344350	0.026*
C114	0.45993 (7)	0.8644 (2)	0.41002 (10)	0.0334 (4)
H114	0.489231	0.910367	0.409651	0.040*
C135	0.31541 (7)	0.3800 (2)	0.64716 (8)	0.0281 (4)
H135	0.304335	0.282456	0.650319	0.034*
C113	0.44331 (8)	0.7215 (2)	0.38745 (11)	0.0378 (5)
H113	0.461097	0.669719	0.371225	0.045*
C126	0.46593 (7)	0.5615 (2)	0.65369 (8)	0.0295 (4)
H126	0.446932	0.511395	0.668847	0.035*
C124	0.55032 (7)	0.6525 (2)	0.66833 (8)	0.0305 (4)
H124	0.588486	0.667102	0.693367	0.037*
C125	0.52219 (7)	0.5787 (3)	0.68975 (8)	0.0391 (5)
H125	0.541310	0.539630	0.729150	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.01180 (11)	0.01177 (11)	0.01257 (11)	0.00131 (8)	0.00597 (9)	−0.00014 (8)
P1	0.01144 (16)	0.01286 (18)	0.01235 (17)	0.00118 (13)	0.00512 (14)	0.00047 (13)
P2	0.01121 (17)	0.01335 (17)	0.01236 (17)	0.00026 (13)	0.00579 (14)	−0.00057 (13)
O1	0.0165 (5)	0.0270 (6)	0.0297 (6)	−0.0022 (4)	0.0136 (5)	−0.0039 (5)
C131	0.0121 (6)	0.0202 (7)	0.0141 (7)	0.0007 (5)	0.0064 (5)	−0.0001 (6)
C116	0.0222 (7)	0.0176 (7)	0.0194 (7)	0.0011 (6)	0.0094 (6)	0.0041 (6)
C115	0.0222 (8)	0.0192 (8)	0.0285 (9)	−0.0038 (6)	0.0071 (7)	0.0058 (7)
C101	0.0136 (6)	0.0162 (7)	0.0136 (6)	0.0031 (5)	0.0062 (5)	−0.0001 (5)
C6	0.0197 (7)	0.0126 (7)	0.0158 (7)	−0.0003 (5)	0.0087 (6)	−0.0014 (5)
C111	0.0126 (6)	0.0174 (7)	0.0162 (7)	0.0016 (5)	0.0054 (6)	0.0045 (6)
C132	0.0149 (7)	0.0206 (7)	0.0159 (7)	0.0020 (6)	0.0067 (6)	−0.0007 (6)
C133	0.0159 (7)	0.0296 (9)	0.0140 (7)	0.0055 (6)	0.0063 (6)	−0.0016 (6)
C11	0.0138 (6)	0.0154 (7)	0.0166 (7)	0.0037 (5)	0.0064 (6)	0.0003 (5)
C106	0.0176 (7)	0.0268 (8)	0.0166 (7)	−0.0019 (6)	0.0087 (6)	0.0005 (6)
C136	0.0253 (8)	0.0214 (8)	0.0199 (8)	−0.0044 (6)	0.0130 (7)	−0.0029 (6)
C4	0.0212 (7)	0.0138 (7)	0.0211 (7)	0.0014 (6)	0.0103 (6)	−0.0035 (6)
C5	0.0207 (7)	0.0166 (7)	0.0182 (7)	0.0045 (6)	0.0114 (6)	−0.0006 (6)
C1	0.0147 (7)	0.0194 (7)	0.0231 (8)	0.0048 (6)	0.0091 (6)	−0.0014 (6)

C12	0.0169 (7)	0.0136 (7)	0.0154 (7)	0.0019 (5)	0.0073 (6)	−0.0007 (5)
C104	0.0205 (7)	0.0261 (8)	0.0133 (7)	0.0040 (6)	0.0049 (6)	−0.0025 (6)
C134	0.0220 (8)	0.0381 (10)	0.0184 (8)	−0.0005 (7)	0.0129 (7)	0.0012 (7)
C3	0.0306 (8)	0.0122 (7)	0.0262 (8)	0.0055 (6)	0.0186 (7)	0.0031 (6)
C105	0.0234 (8)	0.0341 (9)	0.0152 (7)	0.0003 (7)	0.0098 (6)	0.0045 (7)
C103	0.0225 (8)	0.0188 (8)	0.0210 (8)	−0.0023 (6)	0.0044 (6)	−0.0035 (6)
C2	0.0236 (8)	0.0191 (8)	0.0179 (7)	0.0109 (6)	0.0079 (6)	0.0029 (6)
C122	0.0174 (7)	0.0245 (8)	0.0204 (7)	0.0009 (6)	0.0082 (6)	0.0072 (6)
C121	0.0128 (6)	0.0161 (7)	0.0151 (7)	−0.0002 (5)	0.0062 (6)	−0.0021 (5)
C123	0.0169 (7)	0.0254 (8)	0.0306 (9)	−0.0032 (6)	0.0115 (7)	0.0030 (7)
C112	0.0256 (8)	0.0194 (8)	0.0443 (10)	−0.0009 (7)	0.0229 (8)	−0.0022 (7)
C102	0.0227 (8)	0.0162 (7)	0.0186 (7)	−0.0016 (6)	0.0061 (6)	0.0014 (6)
C114	0.0208 (8)	0.0269 (9)	0.0529 (12)	−0.0013 (7)	0.0199 (8)	0.0089 (8)
C135	0.0343 (9)	0.0283 (9)	0.0253 (8)	−0.0090 (7)	0.0183 (8)	0.0001 (7)
C113	0.0334 (10)	0.0276 (9)	0.0685 (14)	0.0006 (8)	0.0380 (10)	−0.0011 (9)
C126	0.0180 (8)	0.0522 (12)	0.0187 (8)	0.0005 (7)	0.0100 (7)	0.0069 (8)
C124	0.0134 (7)	0.0488 (12)	0.0223 (8)	−0.0039 (7)	0.0049 (6)	−0.0058 (8)
C125	0.0184 (8)	0.0780 (16)	0.0159 (8)	0.0017 (9)	0.0057 (7)	0.0067 (9)

Geometric parameters (Å, º)

Mn1—C6	1.7549 (15)	C4—C3	1.428 (2)
Mn1—C5	2.1340 (15)	C4—H4	0.9500
Mn1—C2	2.1353 (15)	C5—C1	1.425 (2)
Mn1—C1	2.1363 (15)	C5—H5	0.9500
Mn1—C3	2.1402 (15)	C1—C2	1.420 (2)
Mn1—C4	2.1417 (15)	C1—H1	0.9500
Mn1—P2	2.1849 (4)	C12—H12A	0.9900
Mn1—P1	2.1968 (4)	C12—H12B	0.9900
P1—C111	1.8422 (15)	C104—C103	1.382 (2)
P1—C101	1.8449 (15)	C104—C105	1.387 (2)
P1—C11	1.8491 (15)	C104—H104	0.9500
P2—C131	1.8362 (15)	C134—C135	1.384 (3)
P2—C121	1.8426 (15)	C134—H134	0.9500
P2—C12	1.8735 (15)	C3—C2	1.414 (2)
O1—C6	1.1753 (19)	C3—H3	0.9500
C131—C136	1.390 (2)	C105—H105	0.9500
C131—C132	1.399 (2)	C103—C102	1.394 (2)
C116—C115	1.390 (2)	C103—H103	0.9500
C116—C111	1.394 (2)	C2—H2	0.9500
C116—H116	0.9500	C122—C123	1.387 (2)
C115—C114	1.377 (3)	C122—C121	1.392 (2)
C115—H115	0.9500	C122—H122	0.9500
C101—C106	1.391 (2)	C121—C126	1.395 (2)
C101—C102	1.395 (2)	C123—C124	1.384 (2)
C111—C112	1.394 (2)	C123—H123	0.9500
C132—C133	1.387 (2)	C112—C113	1.392 (2)
C132—H132	0.9500	C112—H112	0.9500

C133—C134	1.384 (3)	C102—H102	0.9500
C133—H133	0.9500	C114—C113	1.386 (3)
C11—C12	1.538 (2)	C114—H114	0.9500
C11—H11A	0.9900	C135—H135	0.9500
C11—H11B	0.9900	C113—H113	0.9500
C106—C105	1.397 (2)	C126—C125	1.394 (2)
C106—H106	0.9500	C126—H126	0.9500
C136—C135	1.394 (2)	C124—C125	1.385 (3)
C136—H136	0.9500	C124—H124	0.9500
C4—C5	1.413 (2)	C125—H125	0.9500
C6—Mn1—C5	129.47 (6)	C3—C4—H4	126.1
C6—Mn1—C2	127.05 (7)	Mn1—C4—H4	124.6
C5—Mn1—C2	64.92 (6)	C4—C5—C1	108.55 (14)
C6—Mn1—C1	159.90 (7)	C4—C5—Mn1	71.00 (8)
C5—Mn1—C1	39.00 (6)	C1—C5—Mn1	70.59 (8)
C2—Mn1—C1	38.84 (6)	C4—C5—H5	125.7
C6—Mn1—C3	95.48 (7)	C1—C5—H5	125.7
C5—Mn1—C3	64.93 (6)	Mn1—C5—H5	124.3
C2—Mn1—C3	38.63 (6)	C2—C1—C5	107.28 (14)
C1—Mn1—C3	65.12 (6)	C2—C1—Mn1	70.54 (9)
C6—Mn1—C4	96.69 (6)	C5—C1—Mn1	70.41 (8)
C5—Mn1—C4	38.58 (6)	C2—C1—H1	126.4
C2—Mn1—C4	64.95 (6)	C5—C1—H1	126.4
C1—Mn1—C4	65.17 (6)	Mn1—C1—H1	124.3
C3—Mn1—C4	38.95 (6)	C11—C12—P2	109.78 (10)
C6—Mn1—P2	88.66 (5)	C11—C12—H12A	109.7
C5—Mn1—P2	141.86 (4)	P2—C12—H12A	109.7
C2—Mn1—P2	92.74 (5)	C11—C12—H12B	109.7
C1—Mn1—P2	104.44 (4)	P2—C12—H12B	109.7
C3—Mn1—P2	116.81 (5)	H12A—C12—H12B	108.2
C4—Mn1—P2	155.45 (4)	C103—C104—C105	119.74 (15)
C6—Mn1—P1	89.63 (5)	C103—C104—H104	120.1
C5—Mn1—P1	95.25 (4)	C105—C104—H104	120.1
C2—Mn1—P1	143.23 (5)	C135—C134—C133	119.61 (15)
C1—Mn1—P1	106.43 (5)	C135—C134—H134	120.2
C3—Mn1—P1	157.76 (5)	C133—C134—H134	120.2
C4—Mn1—P1	118.99 (4)	C2—C3—C4	107.82 (14)
P2—Mn1—P1	84.865 (16)	C2—C3—Mn1	70.50 (9)
C111—P1—C101	100.52 (7)	C4—C3—Mn1	70.58 (9)
C111—P1—C11	103.23 (7)	C2—C3—H3	126.1
C101—P1—C11	104.03 (6)	C4—C3—H3	126.1
C111—P1—Mn1	120.78 (5)	Mn1—C3—H3	124.4
C101—P1—Mn1	119.63 (5)	C104—C105—C106	120.22 (15)
C11—P1—Mn1	106.49 (5)	C104—C105—H105	119.9
C131—P2—C121	100.10 (7)	C106—C105—H105	119.9
C131—P2—C12	103.53 (7)	C104—C103—C102	119.97 (15)
C121—P2—C12	103.53 (7)	C104—C103—H103	120.0

C131—P2—Mn1	119.22 (5)	C102—C103—H103	120.0
C121—P2—Mn1	117.15 (5)	C3—C2—C1	108.59 (14)
C12—P2—Mn1	111.27 (5)	C3—C2—Mn1	70.87 (9)
C136—C131—C132	118.84 (14)	C1—C2—Mn1	70.62 (9)
C136—C131—P2	119.67 (12)	C3—C2—H2	125.7
C132—C131—P2	121.38 (12)	C1—C2—H2	125.7
C115—C116—C111	121.39 (16)	Mn1—C2—H2	124.4
C115—C116—H116	119.3	C123—C122—C121	121.35 (15)
C111—C116—H116	119.3	C123—C122—H122	119.3
C114—C115—C116	120.18 (16)	C121—C122—H122	119.3
C114—C115—H115	119.9	C122—C121—C126	118.06 (14)
C116—C115—H115	119.9	C122—C121—P2	119.30 (11)
C106—C101—C102	118.46 (14)	C126—C121—P2	122.38 (12)
C106—C101—P1	122.38 (12)	C124—C123—C122	119.97 (16)
C102—C101—P1	119.16 (11)	C124—C123—H123	120.0
O1—C6—Mn1	178.94 (14)	C122—C123—H123	120.0
C112—C111—C116	117.71 (14)	C113—C112—C111	120.92 (16)
C112—C111—P1	119.97 (12)	C113—C112—H112	119.5
C116—C111—P1	122.28 (12)	C111—C112—H112	119.5
C133—C132—C131	120.67 (15)	C103—C102—C101	121.02 (15)
C133—C132—H132	119.7	C103—C102—H102	119.5
C131—C132—H132	119.7	C101—C102—H102	119.5
C134—C133—C132	120.13 (15)	C115—C114—C113	119.48 (16)
C134—C133—H133	119.9	C115—C114—H114	120.3
C132—C133—H133	119.9	C113—C114—H114	120.3
C12—C11—P1	109.07 (10)	C134—C135—C136	120.60 (16)
C12—C11—H11A	109.9	C134—C135—H135	119.7
P1—C11—H11A	109.9	C136—C135—H135	119.7
C12—C11—H11B	109.9	C114—C113—C112	120.30 (18)
P1—C11—H11B	109.9	C114—C113—H113	119.9
H11A—C11—H11B	108.3	C112—C113—H113	119.9
C101—C106—C105	120.59 (15)	C125—C126—C121	120.69 (16)
C101—C106—H106	119.7	C125—C126—H126	119.7
C105—C106—H106	119.7	C121—C126—H126	119.7
C131—C136—C135	120.14 (15)	C123—C124—C125	119.62 (16)
C131—C136—H136	119.9	C123—C124—H124	120.2
C135—C136—H136	119.9	C125—C124—H124	120.2
C5—C4—C3	107.76 (14)	C124—C125—C126	120.22 (17)
C5—C4—Mn1	70.41 (9)	C124—C125—H125	119.9
C3—C4—Mn1	70.47 (9)	C126—C125—H125	119.9
C5—C4—H4	126.1		
C121—P2—C131—C136	−111.18 (13)	C121—P2—C12—C11	134.18 (10)
C12—P2—C131—C136	142.13 (13)	Mn1—P2—C12—C11	7.50 (11)
Mn1—P2—C131—C136	17.93 (14)	C132—C133—C134—C135	−1.0 (2)
C121—P2—C131—C132	64.85 (13)	C5—C4—C3—C2	−0.13 (17)
C12—P2—C131—C132	−41.84 (13)	Mn1—C4—C3—C2	−60.97 (11)
Mn1—P2—C131—C132	−166.05 (10)	C5—C4—C3—Mn1	60.84 (10)

C111—C116—C115—C114	1.3 (3)	C103—C104—C105—C106	−0.1 (3)
C111—P1—C101—C106	−23.06 (14)	C101—C106—C105—C104	0.7 (3)
C11—P1—C101—C106	83.57 (14)	C105—C104—C103—C102	−0.6 (3)
Mn1—P1—C101—C106	−157.83 (11)	C4—C3—C2—C1	0.19 (17)
C111—P1—C101—C102	156.71 (13)	Mn1—C3—C2—C1	−60.84 (11)
C11—P1—C101—C102	−96.66 (13)	C4—C3—C2—Mn1	61.03 (10)
Mn1—P1—C101—C102	21.94 (14)	C5—C1—C2—C3	−0.17 (17)
C115—C116—C111—C112	−1.6 (2)	Mn1—C1—C2—C3	61.00 (11)
C115—C116—C111—P1	176.08 (12)	C5—C1—C2—Mn1	−61.17 (10)
C101—P1—C111—C112	−71.61 (14)	C123—C122—C121—C126	−2.9 (3)
C11—P1—C111—C112	−178.88 (13)	C123—C122—C121—P2	−177.15 (13)
Mn1—P1—C111—C112	62.48 (14)	C131—P2—C121—C122	−163.15 (13)
C101—P1—C111—C116	110.77 (13)	C12—P2—C121—C122	−56.46 (14)
C11—P1—C111—C116	3.50 (14)	Mn1—P2—C121—C122	66.41 (14)
Mn1—P1—C111—C116	−115.15 (12)	C131—P2—C121—C126	22.82 (16)
C136—C131—C132—C133	−0.4 (2)	C12—P2—C121—C126	129.51 (15)
P2—C131—C132—C133	−176.49 (11)	Mn1—P2—C121—C126	−107.62 (14)
C131—C132—C133—C134	1.3 (2)	C121—C122—C123—C124	1.3 (3)
C111—P1—C11—C12	−80.78 (11)	C116—C111—C112—C113	0.9 (3)
C101—P1—C11—C12	174.63 (10)	P1—C111—C112—C113	−176.88 (16)
Mn1—P1—C11—C12	47.38 (11)	C104—C103—C102—C101	0.8 (3)
C102—C101—C106—C105	−0.6 (2)	C106—C101—C102—C103	−0.1 (2)
P1—C101—C106—C105	179.19 (13)	P1—C101—C102—C103	−179.93 (13)
C132—C131—C136—C135	−0.6 (2)	C116—C115—C114—C113	−0.2 (3)
P2—C131—C136—C135	175.51 (13)	C133—C134—C135—C136	0.0 (3)
C3—C4—C5—C1	0.02 (17)	C131—C136—C135—C134	0.9 (3)
Mn1—C4—C5—C1	60.90 (10)	C115—C114—C113—C112	−0.6 (3)
C3—C4—C5—Mn1	−60.88 (10)	C111—C112—C113—C114	0.2 (3)
C4—C5—C1—C2	0.09 (17)	C122—C121—C126—C125	2.0 (3)
Mn1—C5—C1—C2	61.26 (10)	P2—C121—C126—C125	176.09 (16)
C4—C5—C1—Mn1	−61.16 (10)	C122—C123—C124—C125	1.3 (3)
P1—C11—C12—P2	−33.70 (12)	C123—C124—C125—C126	−2.1 (3)
C131—P2—C12—C11	−121.73 (10)	C121—C126—C125—C124	0.5 (3)

Carbonyl*η*⁵-1-chlorocyclopentadienyl)[1,2-bis(diphenylphosphanyl)ethane-*κ*²*P*,*P*′]manganese(I) (compd3b)

Crystal data

[Mn(C₅H₄Cl)(C₂₆H₂₄P₂)(CO)]	$Z = 2$
$M_r = 580.87$	$F(000) = 600$
Triclinic, $P\bar{1}$	$D_x = 1.444$ Mg m⁻³
$a = 8.5739$ (5) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 11.5697$ (8) Å	Cell parameters from 9882 reflections
$c = 14.3909$ (9) Å	$\theta = 2.8–26.4°$
$\alpha = 90.584$ (2)°	$\mu = 0.74$ mm⁻¹
$\beta = 91.958$ (2)°	$T = 100$ K
$\gamma = 110.490$ (2)°	Block, yellow
$V = 1336.07$ (15) Å³	0.08 × 0.06 × 0.03 mm

Data collection

Bruker D8 Venture diffractometer	24803 measured reflections
Radiation source: rotating anode generator, Bruker TXS	5453 independent reflections
	4783 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.035$
Detector resolution: 7.4074 pixels mm⁻¹	$\theta_{max} = 26.4°, \theta_{min} = 3.4°$

Bruker D8 Venture diffractometer

Radiation source: rotating anode generator, Bruker TXS

Detector resolution: 7.4074 pixels mm^{-1}

mix of ω and phi scans

Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)

$T_{min} = 0.702, T_{max} = 0.745$

24803 measured reflections

5453 independent reflections

4783 reflections with $I > 2\sigma(I)$

$R_{int} = 0.035$

$\theta_{max} = 26.4°, \theta_{min} = 3.4°$

$h = -10\rightarrow10$

$k = -14\rightarrow14$

$l = -17\rightarrow17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.063$

$S = 1.04$

5453 reflections

334 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0162P)^2 + 1.2139P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.39$ e Å⁻³

$\Delta\rho_{min} = -0.31$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
C1	1.0229 (2)	0.34942 (15)	0.73902 (12)	0.0150 (3)
C2	1.0240 (2)	0.44703 (16)	0.67950 (12)	0.0167 (4)
H2	0.991655	0.439937	0.615293	0.020*
C3	1.0829 (2)	0.55674 (16)	0.73466 (13)	0.0182 (4)
H3	1.096801	0.637136	0.713528	0.022*
C4	1.1177 (2)	0.52731 (16)	0.82655 (13)	0.0181 (4)
H4	1.158667	0.584157	0.877402	0.022*
C5	1.0807 (2)	0.39815 (16)	0.82915 (12)	0.0163 (3)
H5	1.092513	0.352689	0.881854	0.020*
C6	0.7758 (2)	0.38431 (15)	0.89975 (12)	0.0142 (3)
C10	0.4591 (2)	0.38358 (15)	0.72779 (12)	0.0162 (3)
H10A	0.440451	0.414319	0.665979	0.019*
H10B	0.353400	0.319989	0.745432	0.019*
C20	0.5103 (2)	0.49038 (15)	0.79947 (12)	0.0145 (3)
H20A	0.478560	0.458105	0.862167	0.017*
H20B	0.451857	0.548364	0.784254	0.017*
C101	0.6210 (2)	0.27789 (15)	0.59620 (11)	0.0136 (3)
C102	0.6145 (2)	0.36332 (17)	0.52925 (13)	0.0199 (4)
H102	0.603132	0.438687	0.548400	0.024*
C103	0.6245 (2)	0.33951 (18)	0.43558 (13)	0.0238 (4)

H103	0.619102	0.398221	0.391079	0.029*
C104	0.6423 (2)	0.23037 (18)	0.40645 (13)	0.0226 (4)
H104	0.649041	0.214127	0.342161	0.027*
C105	0.6501 (2)	0.14551 (17)	0.47140 (13)	0.0209 (4)
H105	0.663546	0.071038	0.451739	0.025*
C106	0.6385 (2)	0.16832 (16)	0.56538 (12)	0.0169 (4)
H106	0.642441	0.108580	0.609319	0.020*
C111	0.5230 (2)	0.15693 (15)	0.76603 (11)	0.0134 (3)
C112	0.3588 (2)	0.08479 (16)	0.73993 (12)	0.0177 (4)
H112	0.297722	0.115485	0.696524	0.021*
C113	0.2839 (2)	−0.03117 (17)	0.77674 (13)	0.0217 (4)
H113	0.171758	−0.078974	0.759106	0.026*
C114	0.3732 (2)	−0.07722 (17)	0.83941 (13)	0.0227 (4)
H114	0.321821	−0.156295	0.865012	0.027*
C115	0.5367 (2)	−0.00797 (16)	0.86450 (13)	0.0205 (4)
H115	0.598026	−0.040005	0.906727	0.025*
C116	0.6117 (2)	0.10862 (15)	0.82803 (12)	0.0155 (3)
H116	0.724169	0.155668	0.845491	0.019*
C201	0.7803 (2)	0.67543 (15)	0.90096 (12)	0.0142 (3)
C202	0.6573 (2)	0.69191 (16)	0.95514 (12)	0.0176 (4)
H202	0.543599	0.643118	0.942438	0.021*
C203	0.7001 (2)	0.77943 (16)	1.02769 (12)	0.0195 (4)
H203	0.615553	0.789674	1.064345	0.023*
C204	0.8656 (2)	0.85167 (16)	1.04663 (12)	0.0200 (4)
H204	0.894267	0.912116	1.095531	0.024*
C205	0.9890 (2)	0.83528 (16)	0.99385 (12)	0.0189 (4)
H205	1.102551	0.884176	1.006830	0.023*
C206	0.9466 (2)	0.74759 (15)	0.92222 (12)	0.0166 (3)
H206	1.032014	0.736280	0.886928	0.020*
C211	0.7670 (2)	0.68767 (16)	0.70704 (12)	0.0162 (3)
C212	0.8239 (2)	0.66836 (18)	0.62082 (13)	0.0234 (4)
H212	0.845484	0.594565	0.608844	0.028*
C213	0.8496 (3)	0.7560 (2)	0.55205 (15)	0.0348 (5)
H213	0.887962	0.741590	0.493424	0.042*
C214	0.8195 (3)	0.8640 (2)	0.56870 (17)	0.0367 (5)
H214	0.838136	0.924180	0.521922	0.044*
C215	0.7624 (3)	0.88393 (18)	0.65359 (16)	0.0319 (5)
H215	0.740909	0.957902	0.664957	0.038*
C216	0.7359 (2)	0.79705 (17)	0.72258 (14)	0.0235 (4)
H216	0.696425	0.811922	0.780760	0.028*
Cl1	0.98967 (5)	0.19846 (4)	0.70342 (3)	0.02179 (10)
O1	0.72276 (15)	0.35039 (12)	0.97254 (8)	0.0214 (3)
P1	0.73786 (5)	0.57185 (4)	0.79858 (3)	0.01181 (9)
P2	0.62449 (5)	0.31347 (4)	0.72127 (3)	0.01134 (9)
Mn1	0.85869 (3)	0.43326 (2)	0.79119 (2)	0.01074 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0114 (8)	0.0127 (8)	0.0220 (9)	0.0053 (6)	0.0039 (7)	−0.0012 (7)
C2	0.0127 (8)	0.0224 (9)	0.0164 (8)	0.0076 (7)	0.0054 (7)	0.0016 (7)
C3	0.0105 (8)	0.0156 (9)	0.0281 (10)	0.0034 (7)	0.0079 (7)	0.0042 (7)
C4	0.0093 (8)	0.0180 (9)	0.0257 (10)	0.0034 (7)	−0.0001 (7)	−0.0051 (7)
C5	0.0100 (8)	0.0201 (9)	0.0207 (9)	0.0074 (7)	0.0013 (7)	0.0018 (7)
C6	0.0110 (8)	0.0124 (8)	0.0189 (9)	0.0039 (6)	−0.0023 (7)	−0.0031 (7)
C10	0.0125 (8)	0.0145 (8)	0.0233 (9)	0.0072 (7)	−0.0013 (7)	−0.0024 (7)
C20	0.0112 (8)	0.0131 (8)	0.0200 (9)	0.0051 (6)	0.0024 (7)	−0.0001 (7)
C101	0.0100 (8)	0.0151 (8)	0.0141 (8)	0.0023 (6)	0.0001 (6)	0.0000 (6)
C102	0.0223 (9)	0.0162 (9)	0.0222 (9)	0.0078 (7)	0.0017 (7)	0.0029 (7)
C103	0.0254 (10)	0.0253 (10)	0.0180 (9)	0.0052 (8)	0.0011 (8)	0.0076 (8)
C104	0.0199 (9)	0.0268 (10)	0.0152 (9)	0.0006 (8)	0.0033 (7)	−0.0011 (7)
C105	0.0214 (9)	0.0185 (9)	0.0208 (9)	0.0045 (7)	0.0030 (7)	−0.0041 (7)
C106	0.0179 (9)	0.0153 (8)	0.0174 (9)	0.0055 (7)	0.0008 (7)	0.0015 (7)
C111	0.0145 (8)	0.0117 (8)	0.0142 (8)	0.0045 (6)	0.0041 (6)	−0.0018 (6)
C112	0.0164 (8)	0.0178 (9)	0.0190 (9)	0.0060 (7)	0.0021 (7)	−0.0020 (7)
C113	0.0177 (9)	0.0166 (9)	0.0273 (10)	0.0013 (7)	0.0062 (7)	−0.0039 (7)
C114	0.0254 (10)	0.0136 (9)	0.0267 (10)	0.0029 (7)	0.0109 (8)	0.0031 (7)
C115	0.0258 (10)	0.0180 (9)	0.0201 (9)	0.0103 (8)	0.0049 (7)	0.0032 (7)
C116	0.0153 (8)	0.0140 (8)	0.0168 (9)	0.0046 (7)	0.0030 (7)	−0.0012 (7)
C201	0.0169 (8)	0.0097 (8)	0.0171 (8)	0.0057 (6)	0.0032 (7)	0.0014 (6)
C202	0.0175 (9)	0.0159 (9)	0.0202 (9)	0.0066 (7)	0.0039 (7)	0.0011 (7)
C203	0.0262 (10)	0.0189 (9)	0.0177 (9)	0.0125 (8)	0.0059 (7)	0.0005 (7)
C204	0.0320 (10)	0.0128 (8)	0.0160 (9)	0.0090 (7)	−0.0006 (7)	−0.0005 (7)
C205	0.0193 (9)	0.0129 (8)	0.0222 (9)	0.0031 (7)	−0.0014 (7)	0.0005 (7)
C206	0.0160 (8)	0.0133 (8)	0.0208 (9)	0.0052 (7)	0.0036 (7)	−0.0001 (7)
C211	0.0126 (8)	0.0142 (8)	0.0212 (9)	0.0039 (7)	−0.0019 (7)	0.0028 (7)
C212	0.0235 (10)	0.0257 (10)	0.0240 (10)	0.0117 (8)	0.0049 (8)	0.0073 (8)
C213	0.0311 (11)	0.0466 (14)	0.0299 (11)	0.0164 (10)	0.0094 (9)	0.0188 (10)
C214	0.0287 (11)	0.0300 (12)	0.0480 (14)	0.0056 (9)	−0.0010 (10)	0.0257 (10)
C215	0.0311 (11)	0.0140 (9)	0.0481 (13)	0.0058 (8)	−0.0107 (10)	0.0065 (9)
C216	0.0235 (10)	0.0174 (9)	0.0303 (10)	0.0086 (8)	−0.0053 (8)	−0.0008 (8)
Cl1	0.0177 (2)	0.0171 (2)	0.0321 (2)	0.00805 (17)	0.00126 (18)	−0.00666 (18)
O1	0.0198 (6)	0.0276 (7)	0.0145 (6)	0.0051 (5)	0.0040 (5)	0.0025 (5)
P1	0.0104 (2)	0.0100 (2)	0.0153 (2)	0.00386 (16)	0.00204 (16)	−0.00008 (16)
P2	0.0107 (2)	0.0103 (2)	0.0134 (2)	0.00411 (16)	0.00053 (16)	−0.00034 (15)
Mn1	0.00906 (12)	0.01056 (13)	0.01304 (13)	0.00385 (9)	0.00177 (9)	0.00023 (9)

Geometric parameters (Å, º)

C1—C5	1.411 (2)	C111—C112	1.398 (2)
C1—C2	1.422 (2)	C111—P2	1.8470 (17)
C1—Cl1	1.7372 (17)	C112—C113	1.388 (3)
C1—Mn1	2.1210 (16)	C112—H112	0.9500
C2—C3	1.414 (2)	C113—C114	1.390 (3)

C2—Mn1	2.1497 (17)	C113—H113	0.9500
C2—H2	0.9500	C114—C115	1.382 (3)
C3—C4	1.417 (3)	C114—H114	0.9500
C3—Mn1	2.1460 (17)	C115—C116	1.392 (2)
C3—H3	0.9500	C115—H115	0.9500
C4—C5	1.416 (2)	C116—H116	0.9500
C4—Mn1	2.1435 (17)	C201—C202	1.397 (2)
C4—H4	0.9500	C201—C206	1.398 (2)
C5—Mn1	2.1354 (16)	C201—P1	1.8334 (17)
C5—H5	0.9500	C202—C203	1.394 (2)
C6—O1	1.172 (2)	C202—H202	0.9500
C6—Mn1	1.7547 (17)	C203—C204	1.387 (3)
C10—C20	1.532 (2)	C203—H203	0.9500
C10—P2	1.8679 (16)	C204—C205	1.388 (3)
C10—H10A	0.9900	C204—H204	0.9500
C10—H10B	0.9900	C205—C206	1.385 (2)
C20—P1	1.8464 (16)	C205—H205	0.9500
C20—H20A	0.9900	C206—H206	0.9500
C20—H20B	0.9900	C211—C212	1.393 (3)
C101—C106	1.397 (2)	C211—C216	1.399 (2)
C101—C102	1.401 (2)	C211—P1	1.8486 (17)
C101—P2	1.8391 (17)	C212—C213	1.391 (3)
C102—C103	1.385 (3)	C212—H212	0.9500
C102—H102	0.9500	C213—C214	1.381 (3)
C103—C104	1.386 (3)	C213—H213	0.9500
C103—H103	0.9500	C214—C215	1.378 (3)
C104—C105	1.379 (3)	C214—H214	0.9500
C104—H104	0.9500	C215—C216	1.387 (3)
C105—C106	1.389 (2)	C215—H215	0.9500
C105—H105	0.9500	C216—H216	0.9500
C106—H106	0.9500	P1—Mn1	2.1961 (5)
C111—C116	1.396 (2)	P2—Mn1	2.2024 (5)
C5—C1—C2	109.30 (15)	C111—C116—H116	119.7
C5—C1—Cl1	124.37 (13)	C202—C201—C206	118.35 (16)
C2—C1—Cl1	125.53 (13)	C202—C201—P1	124.29 (13)
C5—C1—Mn1	71.19 (9)	C206—C201—P1	117.25 (12)
C2—C1—Mn1	71.65 (9)	C203—C202—C201	120.47 (16)
Cl1—C1—Mn1	131.49 (9)	C203—C202—H202	119.8
C3—C2—C1	106.50 (15)	C201—C202—H202	119.8
C3—C2—Mn1	70.64 (10)	C204—C203—C202	120.30 (16)
C1—C2—Mn1	69.47 (9)	C204—C203—H203	119.8
C3—C2—H2	126.8	C202—C203—H203	119.8
C1—C2—H2	126.8	C203—C204—C205	119.73 (16)
Mn1—C2—H2	124.8	C203—C204—H204	120.1
C2—C3—C4	108.95 (15)	C205—C204—H204	120.1
C2—C3—Mn1	70.92 (10)	C206—C205—C204	119.97 (17)
C4—C3—Mn1	70.62 (10)	C206—C205—H205	120.0

C2—C3—H3	125.5	C204—C205—H205	120.0
C4—C3—H3	125.5	C205—C206—C201	121.16 (16)
Mn1—C3—H3	124.5	C205—C206—H206	119.4
C5—C4—C3	107.89 (15)	C201—C206—H206	119.4
C5—C4—Mn1	70.37 (9)	C212—C211—C216	118.37 (17)
C3—C4—Mn1	70.81 (10)	C212—C211—P1	120.17 (13)
C5—C4—H4	126.1	C216—C211—P1	121.45 (14)
C3—C4—H4	126.1	C213—C212—C211	120.69 (19)
Mn1—C4—H4	124.4	C213—C212—H212	119.7
C1—C5—C4	107.37 (15)	C211—C212—H212	119.7
C1—C5—Mn1	70.09 (9)	C214—C213—C212	120.2 (2)
C4—C5—Mn1	70.99 (9)	C214—C213—H213	119.9
C1—C5—H5	126.3	C212—C213—H213	119.9
C4—C5—H5	126.3	C215—C214—C213	119.61 (19)
Mn1—C5—H5	124.2	C215—C214—H214	120.2
O1—C6—Mn1	178.60 (15)	C213—C214—H214	120.2
C20—C10—P2	110.55 (11)	C214—C215—C216	120.64 (19)
C20—C10—H10A	109.5	C214—C215—H215	119.7
P2—C10—H10A	109.5	C216—C215—H215	119.7
C20—C10—H10B	109.5	C215—C216—C211	120.43 (19)
P2—C10—H10B	109.5	C215—C216—H216	119.8
H10A—C10—H10B	108.1	C211—C216—H216	119.8
C10—C20—P1	109.42 (11)	C201—P1—C20	103.15 (8)
C10—C20—H20A	109.8	C201—P1—C211	98.82 (8)
P1—C20—H20A	109.8	C20—P1—C211	104.77 (8)
C10—C20—H20B	109.8	C201—P1—Mn1	119.08 (6)
P1—C20—H20B	109.8	C20—P1—Mn1	108.29 (5)
H20A—C20—H20B	108.2	C211—P1—Mn1	120.63 (6)
C106—C101—C102	117.85 (16)	C101—P2—C111	100.44 (7)
C106—C101—P2	120.59 (13)	C101—P2—C10	102.25 (8)
C102—C101—P2	121.36 (13)	C111—P2—C10	103.34 (8)
C103—C102—C101	120.97 (17)	C101—P2—Mn1	119.31 (5)
C103—C102—H102	119.5	C111—P2—Mn1	118.15 (6)
C101—C102—H102	119.5	C10—P2—Mn1	111.06 (6)
C102—C103—C104	120.29 (17)	C6—Mn1—C1	116.64 (7)
C102—C103—H103	119.9	C6—Mn1—C5	91.10 (7)
C104—C103—H103	119.9	C1—Mn1—C5	38.72 (7)
C105—C104—C103	119.59 (17)	C6—Mn1—C4	102.43 (7)
C105—C104—H104	120.2	C1—Mn1—C4	64.57 (7)
C103—C104—H104	120.2	C5—Mn1—C4	38.65 (7)
C104—C105—C106	120.38 (17)	C6—Mn1—C3	139.41 (7)
C104—C105—H105	119.8	C1—Mn1—C3	64.35 (7)
C106—C105—H105	119.8	C5—Mn1—C3	64.67 (7)
C105—C106—C101	120.92 (16)	C4—Mn1—C3	38.57 (7)
C105—C106—H106	119.5	C6—Mn1—C2	154.87 (7)
C101—C106—H106	119.5	C1—Mn1—C2	38.89 (7)
C116—C111—C112	118.62 (16)	C5—Mn1—C2	65.26 (7)
C116—C111—P2	119.43 (13)	C4—Mn1—C2	64.91 (7)

C112—C111—P2	121.95 (13)	C3—Mn1—C2	38.44 (7)
C113—C112—C111	120.76 (17)	C6—Mn1—P1	86.71 (5)
C113—C112—H112	119.6	C1—Mn1—P1	155.95 (5)
C111—C112—H112	119.6	C5—Mn1—P1	143.64 (5)
C112—C113—C114	119.90 (17)	C4—Mn1—P1	106.71 (5)
C112—C113—H113	120.1	C3—Mn1—P1	94.53 (5)
C114—C113—H113	120.1	C2—Mn1—P1	117.20 (5)
C115—C114—C113	120.01 (17)	C6—Mn1—P2	90.06 (5)
C115—C114—H114	120.0	C1—Mn1—P2	99.23 (5)
C113—C114—H114	120.0	C5—Mn1—P2	130.66 (5)
C114—C115—C116	120.16 (17)	C4—Mn1—P2	162.72 (5)
C114—C115—H115	119.9	C3—Mn1—P2	130.52 (5)
C116—C115—H115	119.9	C2—Mn1—P2	98.91 (5)
C115—C116—C111	120.54 (16)	P1—Mn1—P2	85.670 (18)
C115—C116—H116	119.7		
C5—C1—C2—C3	−0.26 (18)	C204—C205—C206—C201	0.8 (3)
Cl1—C1—C2—C3	−170.32 (12)	C202—C201—C206—C205	−1.4 (3)
Mn1—C1—C2—C3	61.31 (11)	P1—C201—C206—C205	174.90 (14)
C5—C1—C2—Mn1	−61.57 (11)	C216—C211—C212—C213	0.2 (3)
Cl1—C1—C2—Mn1	128.37 (13)	P1—C211—C212—C213	−178.66 (15)
C1—C2—C3—C4	0.12 (18)	C211—C212—C213—C214	0.3 (3)
Mn1—C2—C3—C4	60.66 (12)	C212—C213—C214—C215	−0.6 (3)
C1—C2—C3—Mn1	−60.54 (11)	C213—C214—C215—C216	0.4 (3)
C2—C3—C4—C5	0.06 (18)	C214—C215—C216—C211	0.0 (3)
Mn1—C3—C4—C5	60.91 (11)	C212—C211—C216—C215	−0.3 (3)
C2—C3—C4—Mn1	−60.85 (12)	P1—C211—C216—C215	178.47 (14)
C2—C1—C5—C4	0.30 (18)	C202—C201—P1—C20	−6.71 (17)
Cl1—C1—C5—C4	170.50 (12)	C206—C201—P1—C20	177.27 (13)
Mn1—C1—C5—C4	−61.55 (11)	C202—C201—P1—C211	100.82 (15)
C2—C1—C5—Mn1	61.85 (11)	C206—C201—P1—C211	−75.20 (14)
Cl1—C1—C5—Mn1	−127.95 (13)	C202—C201—P1—Mn1	−126.63 (13)
C3—C4—C5—C1	−0.22 (18)	C206—C201—P1—Mn1	57.35 (14)
Mn1—C4—C5—C1	60.98 (11)	C10—C20—P1—C201	−170.00 (12)
C3—C4—C5—Mn1	−61.20 (11)	C10—C20—P1—C211	87.03 (13)
P2—C10—C20—P1	34.87 (15)	C10—C20—P1—Mn1	−42.92 (12)
C106—C101—C102—C103	0.2 (3)	C212—C211—P1—C201	149.94 (15)
P2—C101—C102—C103	175.14 (14)	C216—C211—P1—C201	−28.85 (16)
C101—C102—C103—C104	−0.4 (3)	C212—C211—P1—C20	−103.86 (15)
C102—C103—C104—C105	0.0 (3)	C216—C211—P1—C20	77.36 (16)
C103—C104—C105—C106	0.7 (3)	C212—C211—P1—Mn1	18.37 (17)
C104—C105—C106—C101	−0.9 (3)	C216—C211—P1—Mn1	−160.42 (12)
C102—C101—C106—C105	0.4 (3)	C106—C101—P2—C111	−34.03 (15)
P2—C101—C106—C105	−174.52 (13)	C102—C101—P2—C111	151.20 (14)
C116—C111—C112—C113	1.7 (2)	C106—C101—P2—C10	−140.29 (14)
P2—C111—C112—C113	−178.10 (13)	C102—C101—P2—C10	44.94 (15)
C111—C112—C113—C114	−0.8 (3)	C106—C101—P2—Mn1	96.79 (14)
C112—C113—C114—C115	−0.5 (3)	C102—C101—P2—Mn1	−77.98 (14)

C113—C114—C115—C116	0.8 (3)	C116—C111—P2—C101	117.78 (14)
C114—C115—C116—C111	0.1 (3)	C112—C111—P2—C101	−62.45 (15)
C112—C111—C116—C115	−1.3 (2)	C116—C111—P2—C10	−136.83 (13)
P2—C111—C116—C115	178.45 (13)	C112—C111—P2—C10	42.93 (15)
C206—C201—C202—C203	0.8 (3)	C116—C111—P2—Mn1	−13.77 (15)
P1—C201—C202—C203	−175.16 (13)	C112—C111—P2—Mn1	166.00 (12)
C201—C202—C203—C204	0.3 (3)	C20—C10—P2—C101	−142.21 (12)
C202—C203—C204—C205	−0.9 (3)	C20—C10—P2—C111	113.79 (12)
C203—C204—C205—C206	0.4 (3)	C20—C10—P2—Mn1	−13.86 (13)