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Key indicators

Single-crystal X-ray study
 $T = 120\text{ K}$
 Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 Disorder in main residue
 R factor = 0.025
 wR factor = 0.064
 Data-to-parameter ratio = 14.2

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

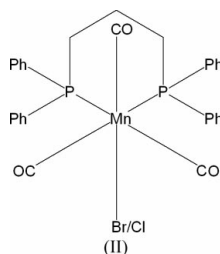
A mixed-halogen tricarbonylmanganese(I) complex: *fac*-[MnBr_{0.3}Cl_{0.7}{Ph₂P(CH₂)₃PPh₂}(CO)₃]

Crystals of the mixed halogen complex, *fac*-(bromo/chloro)-tricarbonyl[1,3-bis(diphenylphosphino)propane]manganese(I), *fac*-[MnBr_{0.3}Cl_{0.7}(C₃₀H₂₆O₃P₂)(CO)₃], were obtained from a prolonged recrystallization attempt of [MnBr{Ph₂P(CH₂)₃PPh₂}(CO)₃] from CHCl₃/hexane solution at 263 K. Common coordinates are found for all but the halogen atoms in the disordered structure, but the Mn–X vectors differ by 3.5 (5)^o and the M–X bond lengths differ by 0.10 (1) Å.

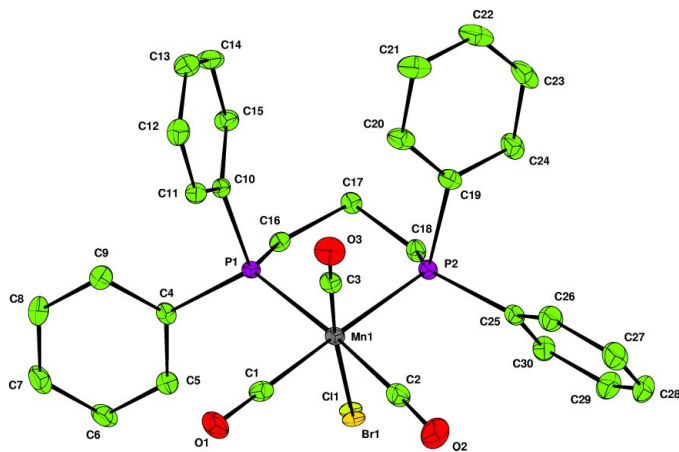
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Comment

In a recent report, we described the synthesis and spectroscopic characterization of *mer*- or *fac*-[MnBrL₂(CO)₃] ($L =$ triorganophosphine) complexes with three compounds $\{L = \frac{1}{2}\text{dppf}$ [dppf = 1,1'-bis(diphenylphosphino)ferrocene], $\frac{1}{2}\text{dppe}$ [dppe = 1,2-bis(diphenylphosphino)ethane] or P(C₆H₄Cl-4)₃] characterized crystallographically (Beckett *et al.*, 2003). Contemporaneously, we also prepared *fac*-[MnBr{Ph₂P(CH₂)₃PPh₂}(CO)₃], (I). The identity of (I) was confirmed by satisfactory elemental and spectroscopic analysis. An attempted (prolonged) recrystallization of (I) from CHCl₃/hexane yielded a few crystals of unusual composition, *viz.* *fac*-[MnBr_{0.3}Cl_{0.7}{Ph₂P(CH₂)₃PPh₂}(CO)₃], (II), with chloride coming from the solvent. The solid-state structure of (II) is described here.



The solid-state structure of (II) is consistent with a 70:30 mixture of *fac*-[MnCl({Ph₂P(CH₂)₃PPh₂}(CO)₃] and *fac*-[MnBr{Ph₂P(CH₂)₃PPh₂}(CO)₃] co-crystallized as a solid solution. The molecular structure of *fac*-[MnCl{Ph₂P(CH₂)₃PPh₂}(CO)₃], (III), is shown in Fig. 1. The d⁶ Mn^I centre in (III) is coordinated by six donor atoms in a (distorted) octahedral environment, with the three CO ligands mutually *fac* and the P atoms of the bidentate 1,3-bis(diphenylphosphino)propane ligand *cis*. The sixth coordination site is occupied by a Cl atom. The angles around Mn involving mutually *cis*-donor atoms and mutually *trans*-donor atoms lie in the ranges 83.3 (3)–96.37 (6) and 174.2 (3)–175.2 (3)^o, respectively. A similar arrangement is adopted for (I), with atomic coordinates of all non-halogen atoms indistinguishable for both the Br and Cl derivatives. However, parameters


Figure 1

View of the structure of (II), showing the atom-numbering scheme. Both possibilities of the disordered halogen site have been shown and H atoms have been omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

associated with the halogen atoms are different. The Mn–X vectors differ by 3.5 (5)° and the M–X bond lengths differ by 0.10 (1) Å. These changes are sufficiently small to accommodate the substitution of [MnBr{Ph₂P(CH₂)₃PPh₂}(CO)₃] for [MnCl{Ph₂P(CH₂)₃PPh₂}(CO)₃] within the same crystal structure. The Mn–P and Mn–C distances are similar to those reported [Mn–P = 2.281 (2)–2.4000 (11) Å and Mn–C = 1.77 (1)–1.953 (9) Å] for related *fac* species such as [MnCl(dppf)(CO)₃] (Onaka *et al.*, 1994), [MnCl(*o*-(Ph₂P)₂-C₆H₄)(CO)₃], [MnCl(*o*-(H₂P)₂C₆H₄)(CO)₃] and [MnBr(dppe)(CO)₃] (Pope & Reid, 1999), [MnCl(Et₂PCH₂CH₂PEt₂)(CO)₃] (Li *et al.*, 1997), and [MnBr(dppf)(CO)₃] and [MnBr(dppe)(CO)₃] (Beckett *et al.*, 2003). Likewise, the Mn–X bond lengths are not significantly different from corresponding bond lengths reported for the complexes cited above [Mn–Cl = 2.386 (2)–2.406 (2) Å and Mn–Br = 2.5068 (8)–2.5273 (7) Å], although the Mn–Br length [2.48 (13) Å] is at the short end of the range, but this may be attributed to the substitution of Cl by Br and crystal packing force constraints. The Mn1–C3 bond *trans* to X is significantly shorter than the Mn1–C1 and Mn1–C2 bonds *trans* to P, consistent with a *trans* influence. The bite angle of the diphenylphosphino-propane ligand is 89.754 (16)° and is close to the average (91.56°) of those in previously determined structures containing this bidentate ligand (Dierke & van Leeuwen, 1999).

Experimental

[MnBr{Ph₂P(CH₂)₃PPh₂}(CO)₃] (I), was prepared by a standard literature procedure (Angelici *et al.*, 1963) in 76% yield (m.p. 483 K). $\nu(\text{CO})$ (cm⁻¹): 2028 (s), 1961 (s), 1909 (s). ³¹P NMR: δ –18.1. Required for C₃₀H₂₆BrMnO₃P₂: C 57.1, H 4.2%; found: C 56.7, H 4.2%. A few orange crystals of the mixed-halide complex (II) were obtained after several months at 263 K from a CHCl₃ solution of (I) layered with hexane.

Crystal data

[MnBr_{0.3}Cl_{0.7}(C₃₀H₂₆O₃P₂)(CO)₃]
 $M_r = 600.18$
 Monoclinic, $P2_1/n$
 $a = 10.0022$ (1) Å
 $b = 20.6821$ (3) Å
 $c = 13.7320$ (2) Å
 $\beta = 106.090$ (1)°
 $V = 2729.41$ (6) Å³
 $Z = 4$

$D_x = 1.461$ Mg m⁻³
 Mo K α radiation
 Cell parameters from 26 531 reflections
 $\theta = 2.9$ –27.5°
 $\mu = 1.14$ mm⁻¹
 $T = 120$ (2) K
 Prism, orange
 0.40 × 0.20 × 0.20 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SORTAV; Blessing, 1997)
 $T_{\min} = 0.659$, $T_{\max} = 0.804$
 9102 measured reflections

4792 independent reflections
 4504 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$
 $\theta_{\text{max}} = 25.0^\circ$
 $h = -11 \rightarrow 11$
 $k = -24 \rightarrow 24$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.025$
 $wR(F^2) = 0.064$
 $S = 1.01$
 4792 reflections
 338 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 2.0712P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.003$
 $\Delta\rho_{\text{max}} = 0.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

Table 1

Selected interatomic distances (Å).

Mn1–C3	1.7820 (19)	Mn1–P1	2.3572 (5)
Mn1–C1	1.8226 (18)	Mn1–Cl1	2.384 (13)
Mn1–C2	1.8317 (19)	Mn1–Br1	2.481 (13)
Mn1–P2	2.3495 (5)		

The structure was found to have a mixed Cl/Br site and the occupancies were refined as free variables with displacement parameter restraints before being fixed in the final refinement. H atoms were found in a difference map, but were then positioned geometrically and included as riding, with C–H = 0.95 and 0.99 Å, and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The coordinates were refined as riding on the parent atom and the occupancy and U_{ij} were fixed.

Data collection: DENZO (Otwinowski & Minor, 1997) and COLLECT (Hooft, 1998); cell refinement: DENZO and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: WinGX (Farrugia, 1999).

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**A mixed-halogen tricarbonylmanganese(I) complex:
fac-[MnBr_{0.3}Cl_{0.7}{Ph₂P(CH₂)₃PPh₂}(CO)₃]**

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fac-(bromo/chloro)tricarbonyl[1,3-bis(diphenylphosphino)propane]manganese(I)

Crystal data

[MnBr_{0.3}Cl_{0.7}(C₃₀H₂₆O₃P₂)(CO)₃]

$M_r = 600.18$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 10.0022$ (1) Å

$b = 20.6821$ (3) Å

$c = 13.7320$ (2) Å

$\beta = 106.090$ (1)°

$V = 2729.41$ (6) Å³

$Z = 4$

$F(000) = 1230$

$D_x = 1.461$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 26531 reflections

$\theta = 2.9$ – 27.5 °

$\mu = 1.14$ mm⁻¹

$T = 120$ K

Prism, orange

$0.40 \times 0.20 \times 0.20$ mm

Data collection

Bruker–Nonius KappaCCD area-detector
diffractometer

Radiation source: Rotating Anode, Bruker
Nonius FR591

Graphite monochromator

Detector resolution: 9.091 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan
(SORTAV; Blessing, 1997)

$T_{\min} = 0.659$, $T_{\max} = 0.804$

9102 measured reflections

4792 independent reflections

4504 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.015$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 3.0$ °

$h = -11 \rightarrow 11$

$k = -24 \rightarrow 24$

$l = -16 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.064$

$S = 1.01$

4792 reflections

338 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 2.0712P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.003$

$\Delta\rho_{\max} = 0.35$ e Å⁻³

$\Delta\rho_{\min} = -0.30$ e Å⁻³

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Mn1	0.03367 (2)	0.111790 (12)	0.265369 (18)	0.01346 (8)	
Br1	-0.1243 (11)	0.0727 (6)	0.3637 (10)	0.0162 (7)	0.30
Cl1	-0.1078 (11)	0.0692 (7)	0.3641 (10)	0.0162 (7)	0.70
O1	-0.17174 (14)	0.07553 (7)	0.07242 (10)	0.0291 (3)	
O2	-0.11973 (16)	0.23550 (7)	0.25914 (11)	0.0379 (4)	
O3	0.20117 (14)	0.17777 (6)	0.15057 (10)	0.0270 (3)	
P1	0.13301 (4)	0.00811 (2)	0.26973 (3)	0.01222 (10)	
P2	0.18760 (4)	0.13453 (2)	0.42487 (3)	0.01407 (10)	
C1	-0.09344 (18)	0.08870 (8)	0.14755 (13)	0.0184 (4)	
C2	-0.05856 (19)	0.18841 (9)	0.26435 (14)	0.0225 (4)	
C3	0.13873 (18)	0.15005 (8)	0.19651 (13)	0.0179 (4)	
C4	0.02199 (17)	-0.05725 (8)	0.20019 (12)	0.0152 (3)	
C5	-0.11268 (18)	-0.06423 (9)	0.20913 (14)	0.0209 (4)	
H5	-0.1482	-0.0335	0.2470	0.025*	
C6	-0.19555 (19)	-0.11584 (9)	0.16293 (15)	0.0243 (4)	
H6	-0.2868	-0.1205	0.1702	0.029*	
C7	-0.1459 (2)	-0.16034 (9)	0.10662 (15)	0.0267 (4)	
H7	-0.2030	-0.1952	0.0745	0.032*	
C8	-0.0129 (2)	-0.15383 (10)	0.09721 (16)	0.0310 (5)	
H8	0.0216	-0.1846	0.0588	0.037*	
C9	0.0714 (2)	-0.10268 (9)	0.14347 (15)	0.0249 (4)	
H9	0.1628	-0.0987	0.1364	0.030*	
C10	0.28325 (17)	0.00516 (8)	0.21874 (12)	0.0142 (3)	
C11	0.26862 (18)	0.03101 (8)	0.12253 (13)	0.0174 (4)	
H11	0.1800	0.0457	0.0834	0.021*	
C12	0.38202 (19)	0.03546 (9)	0.08333 (13)	0.0211 (4)	
H12	0.3705	0.0528	0.0174	0.025*	
C13	0.51196 (19)	0.01480 (9)	0.13984 (14)	0.0242 (4)	
H13	0.5902	0.0193	0.1140	0.029*	
C14	0.52714 (19)	-0.01247 (10)	0.23413 (14)	0.0244 (4)	
H14	0.6158	-0.0275	0.2725	0.029*	
C15	0.41331 (18)	-0.01803 (9)	0.27334 (13)	0.0195 (4)	
H15	0.4243	-0.0377	0.3376	0.023*	
C16	0.19140 (17)	-0.03009 (8)	0.39487 (12)	0.0143 (3)	
H16A	0.1078	-0.0419	0.4162	0.017*	

H16B	0.2396	-0.0708	0.3875	0.017*
C17	0.28795 (17)	0.00913 (8)	0.48050 (12)	0.0154 (3)
H17A	0.3254	-0.0197	0.5393	0.019*
H17B	0.3675	0.0251	0.4576	0.019*
C18	0.21637 (18)	0.06682 (8)	0.51456 (12)	0.0162 (4)
H18A	0.2742	0.0818	0.5814	0.019*
H18B	0.1256	0.0526	0.5229	0.019*
C19	0.36961 (17)	0.15668 (8)	0.43925 (13)	0.0177 (4)
C20	0.43408 (18)	0.14319 (9)	0.36369 (15)	0.0218 (4)
H20	0.3802	0.1276	0.2998	0.026*
C21	0.57690 (19)	0.15236 (9)	0.38088 (17)	0.0284 (4)
H21	0.6198	0.1436	0.3286	0.034*
C22	0.6558 (2)	0.17423 (9)	0.47422 (17)	0.0311 (5)
H22	0.7533	0.1800	0.4863	0.037*
C23	0.5935 (2)	0.18763 (9)	0.54982 (17)	0.0305 (5)
H23	0.6484	0.2025	0.6139	0.037*
C24	0.4510 (2)	0.17953 (9)	0.53306 (15)	0.0248 (4)
H24	0.4087	0.1895	0.5852	0.030*
C25	0.12680 (18)	0.19939 (8)	0.49242 (13)	0.0187 (4)
C26	0.1334 (2)	0.26315 (9)	0.46047 (15)	0.0255 (4)
H26	0.1734	0.2724	0.4068	0.031*
C27	0.0813 (2)	0.31328 (10)	0.50727 (17)	0.0325 (5)
H27	0.0854	0.3566	0.4850	0.039*
C28	0.0240 (2)	0.30034 (10)	0.58568 (16)	0.0341 (5)
H28	-0.0110	0.3347	0.6174	0.041*
C29	0.0174 (2)	0.23756 (11)	0.61824 (16)	0.0322 (5)
H29	-0.0219	0.2288	0.6724	0.039*
C30	0.06850 (19)	0.18705 (9)	0.57143 (14)	0.0238 (4)
H30	0.0634	0.1439	0.5937	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mn1	0.01189 (14)	0.01254 (14)	0.01429 (14)	0.00182 (9)	0.00087 (10)	0.00089 (10)
Br1	0.0096 (18)	0.0209 (10)	0.02039 (18)	0.0001 (11)	0.0081 (11)	-0.0013 (5)
Cl1	0.0096 (18)	0.0209 (10)	0.02039 (18)	0.0001 (11)	0.0081 (11)	-0.0013 (5)
O1	0.0249 (7)	0.0337 (8)	0.0218 (7)	0.0006 (6)	-0.0051 (6)	-0.0025 (6)
O2	0.0377 (8)	0.0247 (8)	0.0431 (9)	0.0176 (7)	-0.0024 (7)	-0.0034 (7)
O3	0.0294 (7)	0.0224 (7)	0.0300 (7)	-0.0015 (6)	0.0094 (6)	0.0093 (6)
P1	0.0107 (2)	0.0124 (2)	0.0130 (2)	0.00051 (16)	0.00238 (16)	0.00040 (16)
P2	0.0138 (2)	0.0114 (2)	0.0154 (2)	0.00051 (16)	0.00128 (17)	-0.00023 (16)
C1	0.0164 (9)	0.0163 (9)	0.0223 (10)	0.0035 (7)	0.0052 (8)	0.0036 (7)
C2	0.0193 (9)	0.0230 (10)	0.0215 (9)	0.0013 (8)	-0.0005 (8)	-0.0014 (8)
C3	0.0167 (9)	0.0142 (8)	0.0188 (9)	0.0036 (7)	-0.0015 (7)	0.0015 (7)
C4	0.0169 (8)	0.0128 (8)	0.0137 (8)	-0.0001 (7)	0.0006 (7)	0.0013 (6)
C5	0.0188 (9)	0.0193 (9)	0.0243 (9)	-0.0012 (7)	0.0053 (7)	-0.0037 (7)
C6	0.0172 (9)	0.0234 (10)	0.0297 (10)	-0.0047 (7)	0.0019 (8)	-0.0015 (8)
C7	0.0270 (10)	0.0176 (9)	0.0297 (10)	-0.0041 (8)	-0.0021 (8)	-0.0044 (8)

C8	0.0320 (11)	0.0244 (10)	0.0361 (11)	-0.0008 (8)	0.0084 (9)	-0.0143 (9)
C9	0.0214 (10)	0.0240 (10)	0.0301 (10)	-0.0009 (8)	0.0085 (8)	-0.0069 (8)
C10	0.0141 (8)	0.0126 (8)	0.0168 (8)	-0.0013 (6)	0.0055 (7)	-0.0021 (7)
C11	0.0162 (9)	0.0177 (9)	0.0173 (9)	0.0018 (7)	0.0029 (7)	-0.0009 (7)
C12	0.0268 (10)	0.0217 (9)	0.0165 (9)	-0.0016 (8)	0.0091 (8)	0.0001 (7)
C13	0.0195 (10)	0.0317 (10)	0.0248 (10)	-0.0021 (8)	0.0116 (8)	-0.0039 (8)
C14	0.0140 (9)	0.0374 (11)	0.0209 (9)	0.0054 (8)	0.0032 (7)	-0.0007 (8)
C15	0.0176 (9)	0.0245 (9)	0.0162 (9)	0.0035 (7)	0.0044 (7)	0.0016 (7)
C16	0.0151 (8)	0.0129 (8)	0.0155 (8)	0.0017 (6)	0.0054 (7)	0.0021 (7)
C17	0.0169 (9)	0.0140 (8)	0.0139 (8)	0.0008 (7)	0.0018 (7)	0.0026 (7)
C18	0.0184 (9)	0.0155 (9)	0.0128 (8)	0.0007 (7)	0.0012 (7)	0.0000 (7)
C19	0.0146 (9)	0.0097 (8)	0.0259 (9)	0.0006 (6)	0.0006 (7)	0.0033 (7)
C20	0.0165 (9)	0.0175 (9)	0.0287 (10)	0.0006 (7)	0.0017 (8)	0.0058 (7)
C21	0.0193 (10)	0.0226 (10)	0.0427 (12)	0.0010 (8)	0.0075 (9)	0.0108 (9)
C22	0.0158 (9)	0.0166 (9)	0.0548 (14)	-0.0016 (7)	-0.0004 (9)	0.0106 (9)
C23	0.0244 (10)	0.0141 (9)	0.0411 (12)	-0.0025 (8)	-0.0106 (9)	-0.0004 (8)
C24	0.0239 (10)	0.0144 (9)	0.0308 (10)	-0.0005 (7)	-0.0011 (8)	-0.0022 (8)
C25	0.0147 (8)	0.0169 (9)	0.0204 (9)	0.0019 (7)	-0.0021 (7)	-0.0042 (7)
C26	0.0239 (10)	0.0192 (9)	0.0305 (10)	0.0012 (8)	0.0027 (8)	-0.0025 (8)
C27	0.0284 (11)	0.0166 (10)	0.0449 (13)	0.0040 (8)	-0.0026 (10)	-0.0059 (9)
C28	0.0285 (11)	0.0305 (11)	0.0385 (12)	0.0096 (9)	0.0012 (9)	-0.0166 (9)
C29	0.0294 (11)	0.0395 (12)	0.0274 (11)	0.0063 (9)	0.0071 (9)	-0.0108 (9)
C30	0.0229 (10)	0.0235 (10)	0.0231 (10)	0.0021 (8)	0.0030 (8)	-0.0051 (8)

Geometric parameters (Å, °)

Mn1—C3	1.7820 (19)	C13—H13	0.9500
Mn1—C1	1.8226 (18)	C14—C15	1.393 (3)
Mn1—C2	1.8317 (19)	C14—H14	0.9500
Mn1—P2	2.3495 (5)	C15—H15	0.9500
Mn1—P1	2.3572 (5)	C16—C17	1.531 (2)
Mn1—Cl1	2.384 (13)	C16—H16A	0.9900
Mn1—Br1	2.481 (13)	C16—H16B	0.9900
O1—C1	1.142 (2)	C17—C18	1.530 (2)
O2—C2	1.142 (2)	C17—H17A	0.9900
O3—C3	1.155 (2)	C17—H17B	0.9900
P1—C10	1.8263 (17)	C18—H18A	0.9900
P1—C16	1.8335 (16)	C18—H18B	0.9900
P1—C4	1.8397 (17)	C19—C20	1.393 (3)
P2—C25	1.8281 (18)	C19—C24	1.402 (3)
P2—C19	1.8340 (17)	C20—C21	1.395 (3)
P2—C18	1.8343 (17)	C20—H20	0.9500
C4—C5	1.393 (2)	C21—C22	1.382 (3)
C4—C9	1.395 (3)	C21—H21	0.9500
C5—C6	1.392 (3)	C22—C23	1.379 (3)
C5—H5	0.9500	C22—H22	0.9500
C6—C7	1.380 (3)	C23—C24	1.389 (3)
C6—H6	0.9500	C23—H23	0.9500

C7—C8	1.378 (3)	C24—H24	0.9500
C7—H7	0.9500	C25—C30	1.390 (3)
C8—C9	1.392 (3)	C25—C26	1.397 (3)
C8—H8	0.9500	C26—C27	1.395 (3)
C9—H9	0.9500	C26—H26	0.9500
C10—C15	1.394 (2)	C27—C28	1.379 (3)
C10—C11	1.395 (2)	C27—H27	0.9500
C11—C12	1.387 (3)	C28—C29	1.381 (3)
C11—H11	0.9500	C28—H28	0.9500
C12—C13	1.384 (3)	C29—C30	1.396 (3)
C12—H12	0.9500	C29—H29	0.9500
C13—C14	1.382 (3)	C30—H30	0.9500
C3—Mn1—C1	90.81 (8)	C14—C13—C12	119.60 (17)
C3—Mn1—C2	88.95 (8)	C14—C13—H13	120.2
C1—Mn1—C2	89.65 (8)	C12—C13—H13	120.2
C3—Mn1—P2	94.32 (6)	C13—C14—C15	120.45 (17)
C1—Mn1—P2	174.68 (6)	C13—C14—H14	119.8
C2—Mn1—P2	91.86 (6)	C15—C14—H14	119.8
C3—Mn1—P1	96.37 (6)	C14—C15—C10	120.31 (16)
C1—Mn1—P1	88.26 (5)	C14—C15—H15	119.8
C2—Mn1—P1	174.31 (6)	C10—C15—H15	119.8
P2—Mn1—P1	89.754 (16)	C17—C16—P1	117.45 (11)
C3—Mn1—C11	175.2 (3)	C17—C16—H16A	107.9
C1—Mn1—C11	91.7 (3)	P1—C16—H16A	107.9
C2—Mn1—C11	87.0 (3)	C17—C16—H16B	107.9
P2—Mn1—C11	83.3 (3)	P1—C16—H16B	107.9
P1—Mn1—C11	87.8 (3)	H16A—C16—H16B	107.2
C3—Mn1—Br1	172.6 (3)	C18—C17—C16	113.51 (14)
C1—Mn1—Br1	90.3 (3)	C18—C17—H17A	108.9
C2—Mn1—Br1	83.7 (3)	C16—C17—H17A	108.9
P2—Mn1—Br1	84.8 (3)	C18—C17—H17B	108.9
P1—Mn1—Br1	91.0 (3)	C16—C17—H17B	108.9
Cl1—Mn1—Br1	3.5 (5)	H17A—C17—H17B	107.7
C10—P1—C16	105.23 (8)	C17—C18—P2	112.94 (12)
C10—P1—C4	102.65 (8)	C17—C18—H18A	109.0
C16—P1—C4	99.18 (7)	P2—C18—H18A	109.0
C10—P1—Mn1	113.99 (5)	C17—C18—H18B	109.0
C16—P1—Mn1	115.99 (5)	P2—C18—H18B	109.0
C4—P1—Mn1	117.75 (5)	H18A—C18—H18B	107.8
C25—P2—C19	102.82 (8)	C20—C19—C24	118.76 (16)
C25—P2—C18	103.41 (8)	C20—C19—P2	121.35 (13)
C19—P2—C18	98.75 (8)	C24—C19—P2	119.31 (14)
C25—P2—Mn1	113.31 (6)	C19—C20—C21	120.69 (18)
C19—P2—Mn1	121.66 (6)	C19—C20—H20	119.7
C18—P2—Mn1	114.42 (6)	C21—C20—H20	119.7
O1—C1—Mn1	178.16 (16)	C22—C21—C20	119.8 (2)
O2—C2—Mn1	176.75 (17)	C22—C21—H21	120.1

O3—C3—Mn1	175.96 (15)	C20—C21—H21	120.1
C5—C4—C9	118.68 (16)	C23—C22—C21	120.18 (18)
C5—C4—P1	119.31 (13)	C23—C22—H22	119.9
C9—C4—P1	121.89 (13)	C21—C22—H22	119.9
C6—C5—C4	120.49 (17)	C22—C23—C24	120.54 (19)
C6—C5—H5	119.8	C22—C23—H23	119.7
C4—C5—H5	119.8	C24—C23—H23	119.7
C7—C6—C5	120.35 (18)	C23—C24—C19	120.05 (19)
C7—C6—H6	119.8	C23—C24—H24	120.0
C5—C6—H6	119.8	C19—C24—H24	120.0
C8—C7—C6	119.62 (17)	C30—C25—C26	119.00 (17)
C8—C7—H7	120.2	C30—C25—P2	122.12 (14)
C6—C7—H7	120.2	C26—C25—P2	118.81 (14)
C7—C8—C9	120.65 (18)	C27—C26—C25	120.06 (19)
C7—C8—H8	119.7	C27—C26—H26	120.0
C9—C8—H8	119.7	C25—C26—H26	120.0
C8—C9—C4	120.22 (17)	C28—C27—C26	120.31 (19)
C8—C9—H9	119.9	C28—C27—H27	119.8
C4—C9—H9	119.9	C26—C27—H27	119.8
C15—C10—C11	118.59 (15)	C27—C28—C29	120.20 (18)
C15—C10—P1	123.33 (13)	C27—C28—H28	119.9
C11—C10—P1	117.96 (13)	C29—C28—H28	119.9
C12—C11—C10	120.71 (16)	C28—C29—C30	119.9 (2)
C12—C11—H11	119.6	C28—C29—H29	120.1
C10—C11—H11	119.6	C30—C29—H29	120.1
C13—C12—C11	120.26 (16)	C25—C30—C29	120.56 (19)
C13—C12—H12	119.9	C25—C30—H30	119.7
C11—C12—H12	119.9	C29—C30—H30	119.7
