Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

A mixed-halogen tricarbonylmanganese(I) complex: *fac*-[$MnBr_{0.3}Cl_{0.7}\{Ph_2P(CH_2)_3PPh_2\}(CO)_3$]

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
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.

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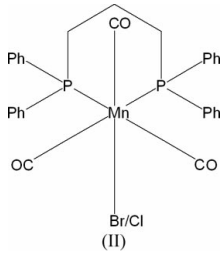
Received 30 July 2004
Accepted 5 August 2004
Online 13 August 2004

Crystals of the mixed halogen complex, *fac*-(bromo/chloro)-tricarbonyl[1,3-bis(diphenylphosphino)propane]manganese(I), *fac*-[$MnBr_{0.3}Cl_{0.7}(C_{30}H_{26}O_3P_2)(CO)_3$], were obtained from a prolonged recrystallization attempt of [$MnBr\{Ph_2P(CH_2)_3PPh_2\}(CO)_3$] from $CHCl_3$/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)° and the M—X bond lengths differ by 0.10 (1) Å.

Comment

In a recent report, we described the synthesis and spectroscopic characterization of *mer*- or *fac*-[$MnBrL_2(CO)_3$] (L = triorganophosphine) complexes with three compounds {L = $\frac{1}{2}$dppf [dppf = 1,1′-bis(diphenylphosphino)ferrocene], $\frac{1}{2}$dppe [dppe = 1,2-bis(diphenylphosphino)ethane] or $P(C_6H_4Cl\text{-}4)_3$} characterized crystallographically (Beckett *et al.*, 2003). Contemporaneously, we also prepared *fac*-[$MnBr\{Ph_2P(CH_2)_3PPh_2\}(CO)_3$], (I). The identity of (I) was confirmed by satisfactory elemental and spectroscopic analysis. An attempted (prolonged) recrystallization of (I) from $CHCl_3$/hexane yielded a few crystals of unusual composition, *viz.* *fac*-[$MnBr_{0.3}Cl_{0.7}\{Ph_2P(CH_2)_3PPh_2\}(CO)_3$], (II), with chloride coming from the solvent. The solid-state structure of (II) is described here.



(II)

The solid-state structure of (II) is consistent with a 70:30 mixture of *fac*-[$MnCl(\{Ph_2P(CH_2)_3PPh_2\}(CO)_3$] and *fac*-[$MnBr\{Ph_2P(CH_2)_3PPh_2\}(CO)_3$] co-crystallized as a solid solution. The molecular structure of *fac*-[$MnCl\{Ph_2P(CH_2)_3PPh_2\}(CO)_3$], (III), is shown in Fig. 1. The d^6 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)°, 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

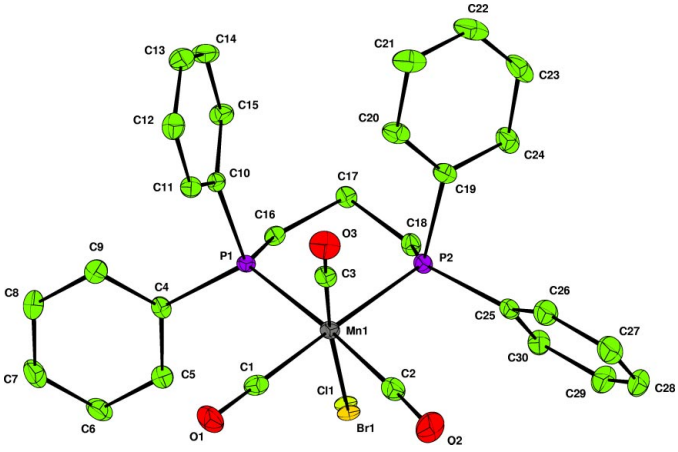


Figure 1
View of the structure of (II), showing the atom-numbering scheme. Both possibilities of the disordered halogen site have been shown and H atoms have been omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

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{$Ph_2P(CH_2)_3PPh_2$}$(CO)_3$] for [MnCl{$Ph_2P(CH_2)_3PPh_2$}$(CO)_3$] 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*-$(Ph_2P)_2C_6H_4$}$(CO)_3$], [MnCl{*o*-$(H_2P)_2C_6H_4$}$(CO)_3$] and [MnBr(dppe)$(CO)_3$] (Pope & Reid, 1999), [MnCl($Et_2PCH_2CH_2PEt_2$)$(CO)_3$] (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 diphenylphosphinopropane 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{$Ph_2P(CH_2)_3PPh_2$}$(CO)_3$], (I), was prepared by a standard literature procedure (Angelici *et al.*, 1963) in 76% yield (m.p. 483 K). ν(CO) (cm^{-1}): 2028 (*s*), 1961 (*s*), 1909 (*s*). ^{31}P NMR: δ −18.1. Required for $C_{30}H_{26}BrMnO_3P_2$: 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 $CHCl_3$ solution of (I) layered with hexane.

Crystal data

$[MnBr_{0.3}Cl_{0.7}(C_{30}H_{26}O_3P_2)(CO)_3]$	D_x = 1.461 Mg m^{-3}
M_r = 600.18	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 26 531 reflections
a = 10.0022 (1) Å	θ = 2.9–27.5°
b = 20.6821 (3) Å	μ = 1.14 mm^{-1}
c = 13.7320 (2) Å	T = 120 (2) K
β = 106.090 (1)°	Prism, orange
V = 2729.41 (6) $Å^3$	0.40 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer	4792 independent reflections
φ and ω scans	4504 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)	R_{int} = 0.015
T_{min} = 0.659, T_{max} = 0.804	θ_{max} = 25.0°
9102 measured reflections	$h = -11 \rightarrow 11$
	$k = -24 \rightarrow 24$
	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 2.0712P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.025	$(\Delta/\sigma)_{max}$ = 0.003
$wR(F^2)$ = 0.064	$\Delta\rho_{max}$ = 0.35 e $Å^{-3}$
S = 1.01	$\Delta\rho_{min}$ = −0.30 e $Å^{-3}$
4792 reflections	
338 parameters	
H-atom parameters constrained	

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_{iso}(H) = 1.2U_{eq}(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: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank the EPSRC for funding the crystallographic facilities.

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supporting information

Acta Cryst. (2004). E**60**, m1245–m1247 [https://doi.org/10.1107/S1600536804019385]

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

Crystal data

$[MnBr_{0.3}Cl_{0.7}(C_{30}H_{26}O_3P_2)(CO)_3]$
$M_r = 600.18$
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) Å^3
$Z = 4$
$F(000) = 1230$
$D_x = 1.461$ 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 × 0.20 × 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 $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.0°$
$h = -11 \rightarrow 11$
$k = -24 \rightarrow 24$
$l = -16 \rightarrow 16$

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{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, º)

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—Cl1	175.2 (3)	C17—C16—H16A	107.9
C1—Mn1—Cl1	91.7 (3)	P1—C16—H16A	107.9
C2—Mn1—Cl1	87.0 (3)	C17—C16—H16B	107.9
P2—Mn1—Cl1	83.3 (3)	P1—C16—H16B	107.9
P1—Mn1—Cl1	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