Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

fac-Dichlorotris(trimethylphosphine)-(trimethylphosphoniomethyl)rhodium(III) chloride/bromide dichloromethane benzene solvate

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Received 8 February 2006
Accepted 15 February 2006

Key indicators

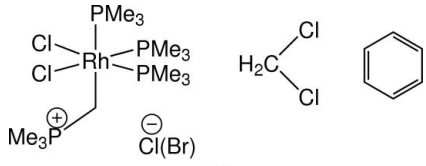
Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
Disorder in solvent or counterion
R factor = 0.030
wR factor = 0.074
Data-to-parameter ratio = 44.8

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

The title complex, $[RhCl_2(C_4H_{11}P)(C_3H_9P)_3](Br_{0.12}/Cl_{0.88})\cdot CH_2Cl_2\cdot C_6H_6$, has an ionic structure with *fac*-octahedral coordination of Rh^{III} in the cation. The anion is a mixture of Cl and Br in a 7:1 ratio.

Comment

The *fac*-$[RhCl_2(CH_2PMe_3)(PMe_3)_3]Cl$ salt has been prepared by Marder, Fultz *et al.* (1987) *via* a reaction of dichloromethane (DCM) with a 16-electron Rh^I complex $[RhCl(PMe_3)_3]$, and characterized by an X-ray crystal structure analysis of its DCM monosolvate, (I*a*). We report here a solvated mixed-anion salt analogue of (I*a*), obtained as a by-product during our ongoing study of PMe_3-containing rhodium–acetylide complexes (Zhu *et al.*, 2006; Rourke *et al.*, 2002; Rourke *et al.*, 1995, 2001; Fyfe *et al.*, 1991; Chow *et al.*, 1989; Zargarian *et al.*, 1989; Marder, Zargarian *et al.*, 1987).



(I)

The asymmetric unit of (I) comprises one *fac*-$[RhCl_2(CH_2PMe_3)(PMe_3)_3]^+$ cation, one halide anion and one DCM molecule in general positions, and two half-molecules of benzene; the benzene rings lie on crystallographic inversion centres. The cation has a somewhat distorted *fac*-octahedral geometry, very similar to that of (I*a*). The Rh—P bond *trans* to C1 is *ca* 0.1 Å longer than the other two, indicating the strong *trans* influence of a σ-bonded C atom in comparison with the chloride ligands. The P1—Me bond lengths in the phosphoniomethyl ligand average 1.793 (2) Å, appreciably shorter than in the phosphine ligands [1.804 (2)–1.837 (2) Å, average 1.818 (9) Å].

Initial treatment of the anion as purely Cl^- gave high residual electron density of 2.4 e Å^{-3} and $R[F^2>2\sigma(F^2)]$ = 0.037. Modelling the disorder between Cl^- and Br^- in a 7:1 ratio resulted in satisfactory refinement. The source of bromide was found to be an impure commercial sample of $RhCl_3\cdot 3H_2O$, which contained a small amount of the bromo analogue, as confirmed later by spectroscopic analysis.

The anion is surrounded by ten H atoms at distances of 2.74–3.17 Å (2.70–3.09 Å using C—H distances normalised to the neutron diffraction value of 1.08 Å). The DCM molecules form hydrogen bonds to both chloro ligands of the cation, especially Cl1 (adjusted H···Cl distances of 2.54 and 2.74 Å).

Experimental

Conversion of impure commercial $RhCl_3{\cdot}2H_2O$ to $Rh(PPh_3)_3Cl/Br$ was followed by reaction with PMe_3 (Jones *et al.*, 1980) which gave the salt, $[Rh(PMe_3)_4]^+{\cdot}Cl^-/Br^-$, which subsequently reacted with DCM solvent to give a very small amount of the title complex. The absence of bromide at the rhodium centre shows that both halides which are coordinated to the metal originate from the DCM and that little, if any, exchange occurs between these and the outer-sphere halide ion.

Crystal data

$[RhCl_2(C_4H_{11}P)(C_3H_9P)_3]$-$(Br_{0.12}/Cl_{0.88}){\cdot}CH_2Cl_2{\cdot}C_6H_6$
M_r = 696.17
Monoclinic, $P2_1/c$
a = 16.949 (3) Å
b = 10.3396 (15) Å
c = 18.424 (3) Å
β = 105.07 (1)°
V = 3117.7 (9) Å^3
Z = 4
D_x = 1.483 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 999 reflections
θ = 12.1–23.7°
μ = 1.34 mm^{-1}
T = 120 (2) K
Block, colourless
0.40 × 0.19 × 0.13 mm

Data collection

Bruker SMART 6K CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.685, T_{max} = 0.845
55018 measured reflections
13203 independent reflections
10300 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 35.0°
$h = -26 \rightarrow 26$
$k = -16 \rightarrow 16$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.074
S = 1.04
13203 reflections
295 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 0.4573P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C14—H141···Cl1	0.99	2.60	3.498 (2)	150
C14—H142···Cl2^{i}	0.99	2.81	3.6455 (19)	142

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Methyl groups were treated as rigid bodies (C—H = 0.98 Å) rotating around the P—C bonds, with a common refined U_{iso} value for the three H atoms. Other H atoms were treated as riding on the attached C atoms [Csp^2—H = 0.95 Å and Csp^3—H = 0.99 Å, with U_{iso}(H) = 1.2U_{eq}(C) and 1.3U_{eq}(C), respectively]. The maximum electron-density peak lies 0.05 Å from the Rh atom

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

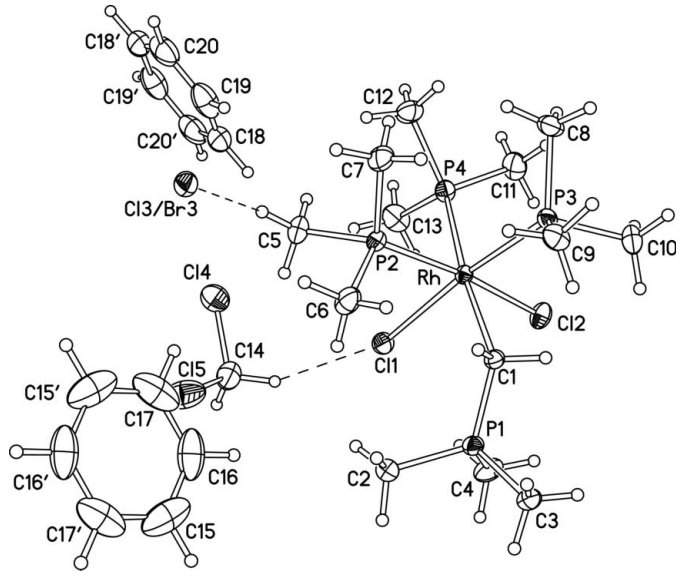


Figure 1
The molecular structure of (I). Atomic displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate hydrogen bonds.

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supporting information

Acta Cryst. (2006). E**62**, m574–m575 [https://doi.org/10.1107/S1600536806005630]

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Hall symbol: -P 2ybc
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$Z = 4$
$F(000) = 1433$
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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 999 reflections
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Graphite monochromator
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ω scans
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$R_{int} = 0.039$
$\theta_{max} = 35.0°$, $\theta_{min} = 2.3°$
$h = -26\rightarrow26$
$k = -16\rightarrow16$
$l = -29\rightarrow29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.074$
$S = 1.04$
13203 reflections
295 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 0.4573P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.23$ e Å^{-3}
$\Delta\rho_{min} = -0.82$ e Å^{-3}

Special details

Experimental. The data collection nominally covered full sphere of reciprocal space, by a combination of 4 sets of ω scans; each set at different φ and/or 2θ angles and each scan (5 sec exposure) covering 0.3° in ω. Crystal to detector distance 4.84 cm.

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Rh	0.229827 (6)	0.536706 (10)	0.289944 (6)	0.01384 (3)	
Cl1	0.18701 (2)	0.61106 (3)	0.159669 (19)	0.02219 (7)	
Cl2	0.14223 (2)	0.70624 (4)	0.31903 (2)	0.02406 (7)	
P1	0.33377 (2)	0.81314 (4)	0.25532 (2)	0.01798 (7)	
P2	0.30304 (2)	0.38566 (3)	0.24615 (2)	0.01641 (7)	
P3	0.28405 (2)	0.48700 (4)	0.41363 (2)	0.01699 (7)	
P4	0.11282 (2)	0.40051 (4)	0.27184 (2)	0.01937 (7)	
C1	0.32553 (8)	0.67881 (13)	0.31290 (8)	0.0166 (2)	
H11	0.3264	0.7153	0.3628	0.022*	
H12	0.3771	0.6298	0.3197	0.022*	
C2	0.37100 (11)	0.77446 (16)	0.17549 (9)	0.0272 (3)	
H21	0.4211	0.7232	0.1917	0.033 (3)*	
H22	0.3827	0.8545	0.1517	0.033 (3)*	
H23	0.3296	0.7245	0.1393	0.033 (3)*	
C3	0.41169 (9)	0.91431 (14)	0.31234 (9)	0.0220 (3)	
H31	0.3916	0.9528	0.3527	0.033 (3)*	
H32	0.4256	0.9831	0.2812	0.033 (3)*	
H33	0.4604	0.8623	0.3342	0.033 (3)*	
C4	0.24409 (10)	0.91192 (15)	0.22570 (10)	0.0282 (3)	
H41	0.2003	0.8618	0.1923	0.037 (3)*	
H42	0.2565	0.9879	0.1988	0.037 (3)*	
H43	0.2265	0.9400	0.2698	0.037 (3)*	
C5	0.25121 (10)	0.31665 (16)	0.15535 (9)	0.0256 (3)	
H51	0.2419	0.3844	0.1169	0.048 (4)*	
H52	0.1987	0.2801	0.1580	0.048 (4)*	
H53	0.2852	0.2483	0.1423	0.048 (4)*	
C6	0.39691 (10)	0.44019 (16)	0.22732 (11)	0.0285 (3)	
H61	0.4214	0.3692	0.2055	0.035 (3)*	
H62	0.4350	0.4682	0.2743	0.035 (3)*	
H63	0.3853	0.5128	0.1919	0.035 (3)*	
C7	0.33736 (11)	0.23993 (15)	0.30053 (9)	0.0275 (3)	
H71	0.3673	0.1850	0.2734	0.036 (3)*	
H72	0.2899	0.1927	0.3079	0.036 (3)*	

H73	0.3734	0.2636	0.3495	0.036 (3)*	
C8	0.25986 (11)	0.33373 (16)	0.45108 (9)	0.0273 (3)	
H81	0.2899	0.3267	0.5041	0.037 (3)*	
H82	0.2756	0.2625	0.4227	0.037 (3)*	
H83	0.2010	0.3294	0.4466	0.037 (3)*	
C9	0.39542 (9)	0.49043 (17)	0.44665 (9)	0.0245 (3)	
H91	0.4147	0.5797	0.4461	0.034 (3)*	
H92	0.4189	0.4371	0.4135	0.034 (3)*	
H93	0.4124	0.4564	0.4980	0.034 (3)*	
C10	0.25548 (11)	0.59942 (17)	0.47770 (9)	0.0287 (3)	
H101	0.1961	0.5974	0.4702	0.043 (4)*	
H102	0.2725	0.6869	0.4680	0.043 (4)*	
H103	0.2824	0.5747	0.5296	0.043 (4)*	
C11	0.04928 (10)	0.42890 (19)	0.33590 (10)	0.0310 (4)	
H111	0.0325	0.5199	0.3330	0.049 (4)*	
H112	0.0804	0.4086	0.3873	0.049 (4)*	
H113	0.0007	0.3736	0.3219	0.049 (4)*	
C12	0.11822 (11)	0.22318 (16)	0.27556 (10)	0.0304 (4)	
H121	0.0628	0.1874	0.2635	0.044 (4)*	
H122	0.1481	0.1957	0.3262	0.044 (4)*	
H123	0.1467	0.1918	0.2390	0.044 (4)*	
C13	0.04018 (10)	0.4277 (2)	0.18184 (10)	0.0325 (4)	
H131	−0.0084	0.3741	0.1782	0.044 (4)*	
H132	0.0653	0.4045	0.1413	0.044 (4)*	
H133	0.0244	0.5191	0.1773	0.044 (4)*	
Cl3	0.42954 (2)	0.11637 (3)	0.144351 (17)	0.02349 (6)	0.88
Br3	0.42954 (2)	0.11637 (3)	0.144351 (17)	0.02349 (6)	0.12
Cl4	0.09222 (3)	0.41111 (5)	−0.03212 (3)	0.03798 (10)	
Cl5	0.24553 (3)	0.52306 (5)	−0.04391 (4)	0.05161 (15)	
C14	0.14745 (12)	0.55584 (18)	−0.03378 (10)	0.0332 (4)	
H141	0.1520	0.6042	0.0135	0.043*	
H142	0.1175	0.6107	−0.0761	0.043*	
C15	0.50603 (17)	0.6315 (2)	0.00684 (14)	0.0600 (8)	
H15	0.5097	0.7230	0.0113	0.072*	
C16	0.44929 (14)	0.5659 (3)	0.03177 (12)	0.0529 (7)	
H16	0.4139	0.6124	0.0547	0.063*	
C17	0.44154 (14)	0.4357 (3)	0.02495 (13)	0.0558 (7)	
H17	0.4005	0.3916	0.0419	0.067*	
C18	0.01271 (16)	0.1256 (2)	0.02329 (13)	0.0475 (6)	
H18	0.0213	0.2127	0.0399	0.057*	
C19	0.07078 (13)	0.0337 (2)	0.05252 (12)	0.0437 (5)	
H19	0.1198	0.0577	0.0884	0.052*	
C20	0.05787 (14)	−0.0927 (2)	0.02988 (13)	0.0457 (5)	
H20	0.0974	−0.1569	0.0507	0.055*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rh	0.01361 (5)	0.01403 (5)	0.01337 (5)	0.00044 (4)	0.00258 (3)	−0.00092 (4)
Cl1	0.02662 (16)	0.02095 (16)	0.01585 (14)	−0.00044 (13)	−0.00012 (12)	0.00117 (12)
Cl2	0.02070 (15)	0.02352 (17)	0.02747 (18)	0.00508 (13)	0.00542 (13)	−0.00617 (14)
P1	0.02141 (17)	0.01436 (15)	0.01723 (16)	−0.00006 (13)	0.00336 (13)	0.00128 (13)
P2	0.01733 (15)	0.01453 (15)	0.01748 (16)	0.00100 (12)	0.00470 (12)	−0.00160 (12)
P3	0.01761 (16)	0.01869 (16)	0.01389 (15)	−0.00203 (13)	0.00270 (12)	0.00031 (12)
P4	0.01625 (15)	0.02318 (18)	0.01866 (17)	−0.00361 (13)	0.00450 (13)	−0.00279 (14)
C1	0.0193 (6)	0.0137 (6)	0.0158 (6)	−0.0001 (5)	0.0028 (5)	0.0004 (5)
C2	0.0393 (9)	0.0225 (7)	0.0218 (7)	−0.0051 (6)	0.0113 (7)	−0.0005 (6)
C3	0.0239 (7)	0.0183 (6)	0.0235 (7)	−0.0036 (5)	0.0056 (6)	−0.0006 (5)
C4	0.0277 (8)	0.0179 (7)	0.0328 (8)	0.0031 (6)	−0.0035 (6)	0.0035 (6)
C5	0.0276 (7)	0.0257 (7)	0.0229 (7)	0.0017 (6)	0.0053 (6)	−0.0072 (6)
C6	0.0261 (7)	0.0244 (8)	0.0400 (9)	−0.0036 (6)	0.0173 (7)	−0.0088 (7)
C7	0.0346 (8)	0.0195 (7)	0.0274 (8)	0.0072 (6)	0.0066 (7)	0.0009 (6)
C8	0.0335 (8)	0.0259 (8)	0.0214 (7)	−0.0085 (6)	0.0051 (6)	0.0057 (6)
C9	0.0197 (7)	0.0307 (8)	0.0201 (7)	−0.0013 (6)	−0.0004 (5)	0.0045 (6)
C10	0.0344 (9)	0.0335 (9)	0.0190 (7)	0.0006 (7)	0.0086 (6)	−0.0047 (6)
C11	0.0242 (7)	0.0394 (9)	0.0333 (9)	−0.0067 (7)	0.0147 (7)	−0.0063 (7)
C12	0.0318 (8)	0.0235 (8)	0.0370 (9)	−0.0085 (7)	0.0111 (7)	−0.0020 (7)
C13	0.0212 (7)	0.0452 (10)	0.0270 (8)	−0.0101 (7)	−0.0012 (6)	0.0005 (7)
Cl3	0.02833 (15)	0.02127 (14)	0.02166 (14)	0.00353 (12)	0.00789 (12)	0.00012 (11)
Br3	0.02833 (15)	0.02127 (14)	0.02166 (14)	0.00353 (12)	0.00789 (12)	0.00012 (11)
Cl4	0.0394 (2)	0.0404 (2)	0.0334 (2)	0.0014 (2)	0.00803 (18)	0.00547 (19)
Cl5	0.0365 (3)	0.0337 (3)	0.0828 (4)	0.0034 (2)	0.0122 (3)	0.0110 (3)
C14	0.0410 (10)	0.0297 (9)	0.0253 (8)	0.0078 (7)	0.0023 (7)	−0.0004 (7)
C15	0.0668 (16)	0.0338 (10)	0.0528 (14)	−0.0045 (11)	−0.0320 (12)	−0.0009 (10)
C16	0.0422 (12)	0.0815 (18)	0.0282 (10)	0.0197 (12)	−0.0029 (8)	−0.0181 (11)
C17	0.0340 (10)	0.091 (2)	0.0351 (11)	−0.0169 (12)	−0.0038 (9)	0.0234 (12)
C18	0.0749 (16)	0.0349 (10)	0.0459 (12)	−0.0133 (11)	0.0392 (12)	−0.0072 (9)
C19	0.0316 (9)	0.0714 (16)	0.0295 (9)	−0.0128 (10)	0.0106 (8)	−0.0020 (10)
C20	0.0464 (12)	0.0562 (13)	0.0441 (11)	0.0171 (10)	0.0288 (10)	0.0166 (10)

Geometric parameters (Å, º)

Rh—C1	2.1475 (14)	C7—H73	0.9799
Rh—P2	2.2695 (4)	C8—H81	0.9800
Rh—P3	2.2832 (5)	C8—H82	0.9800
Rh—P4	2.3840 (5)	C8—H83	0.9801
Rh—Cl1	2.4439 (5)	C9—H91	0.9800
Rh—Cl2	2.4449 (4)	C9—H92	0.9800
P1—C1	1.7751 (14)	C9—H93	0.9799
P1—C2	1.7900 (16)	C10—H101	0.9801
P1—C4	1.7944 (16)	C10—H102	0.9799
P1—C3	1.7946 (15)	C10—H103	0.9801
P2—C6	1.8046 (16)	C11—H111	0.9800

P2—C7	1.8191 (16)	C11—H112	0.9800
P2—C5	1.8208 (16)	C11—H113	0.9800
P3—C10	1.8100 (17)	C12—H121	0.9800
P3—C8	1.8174 (16)	C12—H122	0.9800
P3—C9	1.8267 (16)	C12—H123	0.9799
P4—C13	1.8117 (17)	C13—H131	0.9799
P4—C11	1.8165 (17)	C13—H132	0.9800
P4—C12	1.8362 (18)	C13—H133	0.9800
C1—H11	0.9900	Cl4—C14	1.770 (2)
C1—H12	0.9900	Cl5—C14	1.753 (2)
C2—H21	0.9800	C14—H141	0.9900
C2—H22	0.9801	C14—H142	0.9900
C2—H23	0.9799	C15—C16	1.351 (4)
C3—H31	0.9799	C15—C17^{i}	1.373 (4)
C3—H32	0.9800	C15—H15	0.9500
C3—H33	0.9799	C16—C17	1.356 (4)
C4—H41	0.9799	C16—H16	0.9499
C4—H42	0.9800	C17—C15^{i}	1.373 (4)
C4—H43	0.9799	C17—H17	0.9499
C5—H51	0.9799	C18—C19	1.373 (3)
C5—H52	0.9800	C18—C20^{ii}	1.377 (3)
C5—H53	0.9800	C18—H18	0.9500
C6—H61	0.9799	C19—C20	1.372 (3)
C6—H62	0.9800	C19—H19	0.9500
C6—H63	0.9800	C20—C18^{ii}	1.378 (3)
C7—H71	0.9800	C20—H20	0.9499
C7—H72	0.9799		

C1—Rh—P2	94.94 (4)	H61—C6—H62	109.5
C1—Rh—P3	82.53 (4)	P2—C6—H63	109.5
P2—Rh—P3	94.848 (17)	H61—C6—H63	109.5
C1—Rh—P4	171.86 (4)	H62—C6—H63	109.5
P2—Rh—P4	93.191 (18)	P2—C7—H71	109.5
P3—Rh—P4	96.375 (16)	P2—C7—H72	109.5
C1—Rh—Cl1	89.68 (4)	H71—C7—H72	109.5
P2—Rh—Cl1	85.269 (16)	P2—C7—H73	109.5
P3—Rh—Cl1	172.191 (14)	H71—C7—H73	109.5
P4—Rh—Cl1	91.412 (16)	H72—C7—H73	109.5
C1—Rh—Cl2	86.38 (4)	P3—C8—H81	109.5
P2—Rh—Cl2	172.141 (14)	P3—C8—H82	109.5
P3—Rh—Cl2	93.005 (16)	H81—C8—H82	109.5
P4—Rh—Cl2	85.625 (18)	P3—C8—H83	109.5
Cl1—Rh—Cl2	86.992 (16)	H81—C8—H83	109.5
C1—P1—C2	114.56 (7)	H82—C8—H83	109.5
C1—P1—C4	115.79 (8)	P3—C9—H91	109.5
C2—P1—C4	109.20 (9)	P3—C9—H92	109.5
C1—P1—C3	105.46 (7)	H91—C9—H92	109.5
C2—P1—C3	104.37 (8)	P3—C9—H93	109.5

C4—P1—C3	106.41 (8)	H91—C9—H93	109.5
C6—P2—C7	101.13 (8)	H92—C9—H93	109.5
C6—P2—C5	100.64 (8)	P3—C10—H101	109.5
C7—P2—C5	100.96 (8)	P3—C10—H102	109.5
C6—P2—Rh	116.37 (6)	H101—C10—H102	109.5
C7—P2—Rh	120.02 (6)	P3—C10—H103	109.5
C5—P2—Rh	114.74 (5)	H101—C10—H103	109.5
C10—P3—C8	100.80 (8)	H102—C10—H103	109.5
C10—P3—C9	101.47 (8)	P4—C11—H111	109.5
C8—P3—C9	101.90 (8)	P4—C11—H112	109.5
C10—P3—Rh	113.57 (6)	H111—C11—H112	109.5
C8—P3—Rh	120.21 (6)	P4—C11—H113	109.5
C9—P3—Rh	116.16 (5)	H111—C11—H113	109.5
C13—P4—C11	101.13 (9)	H112—C11—H113	109.5
C13—P4—C12	101.79 (9)	P4—C12—H121	109.5
C11—P4—C12	99.75 (9)	P4—C12—H122	109.5
C13—P4—Rh	112.28 (6)	H121—C12—H122	109.5
C11—P4—Rh	115.20 (6)	P4—C12—H123	109.5
C12—P4—Rh	123.57 (6)	H121—C12—H123	109.5
P1—C1—Rh	126.18 (7)	H122—C12—H123	109.5
P1—C1—H11	105.8	P4—C13—H131	109.5
Rh—C1—H11	105.8	P4—C13—H132	109.5
P1—C1—H12	105.8	H131—C13—H132	109.5
Rh—C1—H12	105.8	P4—C13—H133	109.5
H11—C1—H12	106.2	H131—C13—H133	109.5
P1—C2—H21	109.5	H132—C13—H133	109.5
P1—C2—H22	109.5	Cl5—C14—Cl4	111.03 (10)
H21—C2—H22	109.5	Cl5—C14—H141	109.4
P1—C2—H23	109.5	Cl4—C14—H141	109.4
H21—C2—H23	109.5	Cl5—C14—H142	109.4
H22—C2—H23	109.5	Cl4—C14—H142	109.5
P1—C3—H31	109.5	H141—C14—H142	108.0
P1—C3—H32	109.5	C16—C15—C17^{i}	119.2 (2)
H31—C3—H32	109.5	C16—C15—H15	120.4
P1—C3—H33	109.5	C17^{i}—C15—H15	120.4
H31—C3—H33	109.5	C15—C16—C17	121.8 (2)
H32—C3—H33	109.5	C15—C16—H16	119.1
P1—C4—H41	109.5	C17—C16—H16	119.1
P1—C4—H42	109.5	C16—C17—C15^{i}	119.0 (2)
H41—C4—H42	109.5	C16—C17—H17	120.5
P1—C4—H43	109.5	C15^{i}—C17—H17	120.5
H41—C4—H43	109.5	C19—C18—C20^{ii}	120.6 (2)
H42—C4—H43	109.5	C19—C18—H18	119.7
P2—C5—H51	109.5	C20^{ii}—C18—H18	119.7
P2—C5—H52	109.5	C20—C19—C18	119.9 (2)
H51—C5—H52	109.5	C20—C19—H19	120.1
P2—C5—H53	109.5	C18—C19—H19	120.0
H51—C5—H53	109.5	C19—C20—C18^{ii}	119.5 (2)

H52—C5—H53	109.5	C19—C20—H20	120.2
P2—C6—H61	109.5	C18^{ii}—C20—H20	120.3
P2—C6—H62	109.5		
Cl1—Rh—C1—P1	14.80 (9)	Rh—C1—P1—C3	167.66 (9)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H141···Cl1	0.99	2.60	3.498 (2)	150
C14—H142···Cl2^{iii}	0.99	2.81	3.6455 (19)	142

Symmetry code: (iii) *x*, −*y*+3/2, *z*−1/2.