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Chloridobis[2-(4-fluoroanilino)tropon-ato-κ^2N,O](triphenylphosphine-κP)-rhodium(III)

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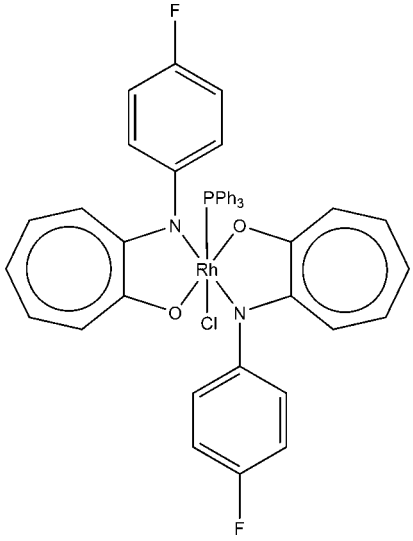
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.064; data-to-parameter ratio = 16.6.

In the title complex, $[Rh(C_{13}H_9NOF)_2Cl(C_{18}H_{15}P)]$, the two 2-(4-fluorophenylamino)troponate groups chelate the Rh^{III} atom and the four coordinating atoms are disposed around it as a square in a *trans* manner. The Cl and P atoms occupy axial positions of the octahedral coordination geometry. The crystal structure shows weak intra- and intermolecular interactions.

Related literature

For general background, see: Crous *et al.* (2005); Otto & Roodt (2004); Roodt *et al.* (2003); Otto & Roodt (2002). For related diketonato complexes, see: Janse van Rensburg & Roodt (2006); Janse van Rensburg *et al.* (2006); Das *et al.* (2002). For the uncoordinated ligand, see: Steyl (2007).



Experimental

Crystal data

$[Rh(C_{13}H_9NOF)_2Cl(C_{18}H_{15}P)]$
M_r = 829.05
Triclinic, $P\overline{1}$
a = 9.4681 (4) Å
b = 10.5333 (5) Å
c = 19.5749 (9) Å
α = 100.552 (2)°
β = 91.904 (2)°
γ = 107.430 (2)°
V = 1822.98 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 100 (2) K
0.35 × 0.35 × 0.06 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.808, T_{max} = 0.963
50714 measured reflections
7924 independent reflections
7289 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.064
S = 1.05
7924 reflections
478 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C116—H116···Cl	0.95	2.83	3.579 (2)	137
C17—H17···F14^{i}	0.95	2.39	3.325 (2)	167
C27—H27···F24^{ii}	0.95	2.63	3.541 (2)	162

Symmetry codes: (i) $x+1, y+1, z$; (ii) $x-1, y-1, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg Putz, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2354).

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supplementary materials

Acta Cryst. (2007). E**63**, m2968-m2969 [**doi:10.1107/S1600536807053755**]

Chloridobis[2-(4-fluoroanilino)troponato-κ^2N,O](triphenylphosphine-κP)rhodium(III)

G. Steyl

Comment

Rhodium(III) complexes play a vital role in catalytic processes applied in industry today (Crous *et al.*, 2005; Otto & Roodt, 2004), with rhodium systems being investigated for a wide variety of catalytic activities (Roodt *et al.*, 2003; Otto & Roodt, 2002). The title complex, (I), is a possible by-product in these systems where diketonato or acetato ligands might be in use. A similar system have been reported for O,*O*-diketonato Rh(III) complexes (Das *et al.*, 2002), however the coordination mode differs with one of the diketonato oxygen atoms coordinated *via* an apical position. The title complex is the first example of a N,*O*-bidentate Rh(III) complex with a triphenylphosphane and halogen moiety, see Fig. 1.

The distortion of the octahedral geometry about the Rh(III) metal centre can be observed from the slight deviation from linearity of the O—Rh—O and N—Rh—N bond angles of the complex, see Table 1. A significant distortion of the cycloheptatriene moeities is observed as these units are twisted away from the apical triphenylphosphane ligand. The distortion of the seven membered rings are also evidant in the torsion angles of the bidentate ligand, Table 1, which differ by 7 ° for the respective units. The free ligand had a similar but smaller torsional change for the O—C—C—N unit (Steyl, 2007).

The effect of weak intra- and intermolecular interactions play a significant role in determining the packing mode of the title complex. Weak intra- and intermolecular hydrogen bonds are formed in the system with the halogen atoms contributing to the solid state ordering, see Table 2. Intercalation is observed between symmetry associated cycloheptatriene rings; C11···C17 and C11···C17 [$-x$, $1-y$, $-z$] and C21···C27 and C21···C27 [$-x$, $1-y$, $1-z$], in the order of 3.282 (2) and 3.534 (6) Å respectively.

Experimental

The title complex was obtained during the attempted synthesis of the [Rh((N-4-FPh)Trop)CO(PPh_3)] derivative, due to the excess of ligands oxidation of the Rh(I) centre occurred. On evaporation of the acetone; crystals suitable for X-Ray crystallography was obtained.

Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.95 Å and with U_{iso}(H) = 1.2 times U_{eq}(C aromatic).

Figures

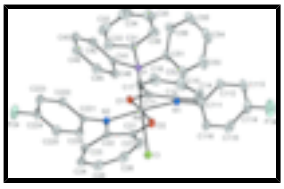


Fig. 1. : Representation of the title compound (I), showing the numbering scheme and displacement ellipsoids (50% probability).

Chloridobis[2-(4-fluoroanilino)troponato- κ^2N,O](triphenylphosphine-κP)rhodium(III)

Crystal data

$[Rh(C_{13}H_9NOF)_2Cl(C_{18}H_{15}P)]$	$Z = 2$
$M_r = 829.05$	$F_{000} = 844$
Triclinic, $P\overline{1}$	$D_x = 1.510$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.4681$ (4) Å	Cell parameters from 9643 reflections
$b = 10.5333$ (5) Å	$\theta = 2.4$–$28.3°$
$c = 19.5749$ (9) Å	$\mu = 0.64$ mm^{-1}
$\alpha = 100.552$ (2)°	$T = 100$ (2) K
$\beta = 91.904$ (2)°	Plate, red
$\gamma = 107.430$ (2)°	0.35 × 0.35 × 0.06 mm
$V = 1822.98$ (14) Å^3	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	7924 independent reflections
Radiation source: fine-focus sealed tube	7289 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.039$
Detector resolution: 512 pixels mm^{-1}	$\theta_{max} = 27.0°$
$T = 100(2)$ K	$\theta_{min} = 2.1°$
phi and ω scans	$h = -11 \rightarrow 12$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$k = -13 \rightarrow 13$
$T_{min} = 0.808$, $T_{max} = 0.963$	$l = -24 \rightarrow 24$
50714 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.025$	H-atom parameters constrained
$wR(F^2) = 0.064$	$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2 + 1.3992P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
7924 reflections	$\Delta\rho_{max} = 0.62$ e Å^{-3}
478 parameters	$\Delta\rho_{min} = -0.63$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Rh	0.077509 (14)	0.273280 (12)	0.269392 (6)	0.01352 (5)
Cl	−0.10642 (5)	0.39378 (4)	0.28114 (2)	0.01912 (9)
P	0.23870 (5)	0.15092 (4)	0.25259 (2)	0.01517 (9)
F24	0.63836 (13)	0.86999 (12)	0.37281 (7)	0.0363 (3)
O2	−0.02742 (14)	0.16654 (12)	0.33902 (6)	0.0188 (2)
O1	0.18050 (13)	0.39257 (11)	0.20541 (6)	0.0155 (2)
F14	−0.48903 (18)	−0.31325 (15)	0.15354 (9)	0.0599 (4)
N1	−0.03774 (16)	0.17037 (14)	0.17478 (7)	0.0163 (3)
N2	0.18529 (16)	0.39043 (14)	0.36101 (7)	0.0155 (3)
C41	0.36683 (19)	0.16472 (17)	0.32757 (9)	0.0172 (3)
C21	0.00897 (19)	0.22668 (18)	0.40479 (9)	0.0178 (3)
C226	0.2743 (2)	0.61971 (18)	0.33940 (9)	0.0194 (4)
H226	0.1770	0.6091	0.3202	0.023*
C24	0.1255 (2)	0.4292 (2)	0.54940 (9)	0.0227 (4)
H24	0.1666	0.5060	0.5861	0.027*
C116	−0.2632 (2)	0.0362 (2)	0.21465 (10)	0.0245 (4)
H116	−0.2582	0.1118	0.2507	0.029*
C12	−0.00746 (19)	0.23929 (17)	0.12344 (9)	0.0166 (3)
C25	0.0302 (2)	0.3155 (2)	0.56990 (9)	0.0258 (4)
H25	0.0207	0.3223	0.6185	0.031*
C46	0.3023 (2)	0.12251 (18)	0.38602 (9)	0.0201 (4)
H46	0.1971	0.0920	0.3857	0.024*
C27	−0.0616 (2)	0.1570 (2)	0.45422 (10)	0.0234 (4)
H27	−0.1280	0.0688	0.4356	0.028*
C22	0.12562 (19)	0.35789 (17)	0.41819 (9)	0.0163 (3)
C56	0.2348 (2)	−0.11511 (19)	0.20036 (10)	0.0261 (4)

H56	0.3302	−0.0748	0.1863	0.031*
C23	0.1691 (2)	0.44731 (18)	0.48484 (9)	0.0190 (3)
H23	0.2394	0.5331	0.4843	0.023*
C42	0.5211 (2)	0.20584 (18)	0.32832 (9)	0.0203 (4)
H42	0.5666	0.2333	0.2886	0.024*
C224	0.5275 (2)	0.75131 (19)	0.36894 (10)	0.0243 (4)
C52	0.0157 (2)	−0.09324 (19)	0.25376 (10)	0.0249 (4)
H52	−0.0397	−0.0384	0.2760	0.030*
C51	0.1532 (2)	−0.03287 (17)	0.23153 (9)	0.0202 (4)
C221	0.30347 (19)	0.51321 (16)	0.36373 (8)	0.0157 (3)
C31	0.3499 (2)	0.19638 (18)	0.18167 (9)	0.0194 (4)
C13	−0.1042 (2)	0.20736 (18)	0.06111 (9)	0.0221 (4)
H13	−0.1985	0.1425	0.0616	0.027*
C11	0.12681 (19)	0.35670 (17)	0.14058 (9)	0.0167 (3)
C45	0.3905 (2)	0.12466 (19)	0.44454 (10)	0.0239 (4)
H45	0.3456	0.0970	0.4843	0.029*
C223	0.5605 (2)	0.64715 (19)	0.39194 (10)	0.0260 (4)
H223	0.6592	0.6571	0.4090	0.031*
C32	0.4651 (2)	0.31947 (19)	0.19284 (10)	0.0245 (4)
H32	0.4851	0.3784	0.2374	0.029*
C55	0.1765 (3)	−0.2557 (2)	0.18998 (10)	0.0334 (5)
H55	0.2318	−0.3111	0.1683	0.040*
C15	0.0404 (3)	0.3479 (2)	−0.01873 (10)	0.0322 (5)
H15	0.0358	0.3604	−0.0655	0.039*
C36	0.3158 (2)	0.1156 (2)	0.11458 (10)	0.0261 (4)
H36	0.2340	0.0343	0.1056	0.031*
C26	−0.0507 (2)	0.1957 (2)	0.52714 (10)	0.0271 (4)
H26	−0.1080	0.1287	0.5503	0.032*
C16	0.1687 (2)	0.4232 (2)	0.02335 (10)	0.0293 (4)
H16	0.2431	0.4798	0.0012	0.035*
C225	0.3870 (2)	0.74156 (19)	0.34297 (10)	0.0234 (4)
H225	0.3675	0.8160	0.3279	0.028*
C17	0.2049 (2)	0.42846 (18)	0.09351 (9)	0.0211 (4)
H17	0.2987	0.4916	0.1124	0.025*
C43	0.6089 (2)	0.20682 (19)	0.38693 (10)	0.0246 (4)
H43	0.7141	0.2349	0.3871	0.029*
C14	−0.0825 (2)	0.2557 (2)	0.00036 (10)	0.0271 (4)
H14	−0.1651	0.2202	−0.0341	0.033*
C222	0.4466 (2)	0.52674 (18)	0.38975 (9)	0.0210 (4)
H222	0.4666	0.4537	0.4060	0.025*
C54	0.0390 (3)	−0.3149 (2)	0.21096 (10)	0.0347 (5)
H54	−0.0008	−0.4111	0.2032	0.042*
C34	0.5184 (3)	0.2719 (3)	0.07349 (11)	0.0379 (5)
H34	0.5779	0.2961	0.0369	0.045*
C44	0.5440 (2)	0.16710 (19)	0.44505 (10)	0.0251 (4)
H44	0.6044	0.1689	0.4852	0.030*
C114	−0.3806 (2)	−0.1929 (2)	0.15728 (12)	0.0373 (5)
C113	−0.2799 (2)	−0.1844 (2)	0.10845 (11)	0.0326 (5)
H113	−0.2876	−0.2601	0.0720	0.039*

C112	−0.1662 (2)	−0.06303 (18)	0.11317 (10)	0.0236 (4)
H112	−0.0938	−0.0556	0.0804	0.028*
C111	−0.1585 (2)	0.04800 (17)	0.16608 (9)	0.0193 (4)
C35	0.4009 (3)	0.1537 (2)	0.06111 (11)	0.0346 (5)
H35	0.3779	0.0978	0.0157	0.041*
C115	−0.3749 (2)	−0.0861 (2)	0.21045 (11)	0.0334 (5)
H115	−0.4462	−0.0957	0.2438	0.040*
C33	0.5504 (2)	0.3561 (2)	0.13909 (11)	0.0332 (5)
H33	0.6305	0.4386	0.1472	0.040*
C53	−0.0411 (3)	−0.2349 (2)	0.24327 (10)	0.0319 (5)
H53	−0.1351	−0.2761	0.2584	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rh	0.01308 (7)	0.01306 (7)	0.01213 (7)	0.00142 (5)	−0.00088 (5)	0.00165 (5)
Cl	0.0173 (2)	0.0206 (2)	0.0185 (2)	0.00600 (16)	0.00075 (15)	0.00159 (15)
P	0.0166 (2)	0.0136 (2)	0.0138 (2)	0.00334 (17)	−0.00083 (16)	0.00194 (16)
F24	0.0266 (6)	0.0267 (6)	0.0439 (7)	−0.0104 (5)	−0.0072 (5)	0.0113 (5)
O2	0.0186 (6)	0.0192 (6)	0.0148 (6)	0.0003 (5)	−0.0003 (5)	0.0035 (5)
O1	0.0177 (6)	0.0139 (5)	0.0137 (6)	0.0032 (5)	−0.0001 (4)	0.0024 (4)
F14	0.0449 (9)	0.0368 (8)	0.0716 (11)	−0.0232 (7)	0.0016 (8)	0.0066 (7)
N1	0.0155 (7)	0.0150 (7)	0.0155 (7)	0.0021 (6)	−0.0008 (5)	0.0006 (5)
N2	0.0146 (7)	0.0149 (7)	0.0149 (7)	0.0022 (6)	−0.0023 (5)	0.0020 (5)
C41	0.0185 (8)	0.0137 (8)	0.0184 (8)	0.0056 (7)	−0.0025 (7)	0.0005 (6)
C21	0.0145 (8)	0.0213 (9)	0.0178 (8)	0.0058 (7)	−0.0005 (6)	0.0046 (7)
C226	0.0170 (8)	0.0211 (9)	0.0180 (8)	0.0034 (7)	−0.0024 (7)	0.0040 (7)
C24	0.0233 (9)	0.0288 (10)	0.0169 (8)	0.0124 (8)	−0.0010 (7)	0.0005 (7)
C116	0.0175 (9)	0.0286 (10)	0.0222 (9)	0.0010 (8)	−0.0018 (7)	0.0032 (7)
C12	0.0182 (8)	0.0161 (8)	0.0154 (8)	0.0072 (7)	0.0016 (6)	−0.0001 (6)
C25	0.0234 (10)	0.0415 (11)	0.0145 (8)	0.0116 (9)	0.0030 (7)	0.0078 (8)
C46	0.0189 (9)	0.0197 (9)	0.0208 (9)	0.0056 (7)	0.0000 (7)	0.0030 (7)
C27	0.0187 (9)	0.0264 (9)	0.0222 (9)	0.0015 (7)	0.0003 (7)	0.0074 (7)
C22	0.0144 (8)	0.0190 (8)	0.0167 (8)	0.0069 (7)	−0.0003 (6)	0.0041 (6)
C56	0.0360 (11)	0.0221 (9)	0.0203 (9)	0.0113 (8)	−0.0059 (8)	0.0021 (7)
C23	0.0190 (9)	0.0189 (8)	0.0183 (8)	0.0062 (7)	−0.0010 (7)	0.0022 (7)
C42	0.0209 (9)	0.0186 (8)	0.0207 (9)	0.0058 (7)	0.0012 (7)	0.0027 (7)
C224	0.0226 (9)	0.0197 (9)	0.0229 (9)	−0.0042 (7)	−0.0017 (7)	0.0039 (7)
C52	0.0294 (10)	0.0190 (9)	0.0222 (9)	0.0023 (8)	−0.0062 (8)	0.0046 (7)
C51	0.0269 (10)	0.0135 (8)	0.0175 (8)	0.0043 (7)	−0.0074 (7)	0.0016 (6)
C221	0.0165 (8)	0.0146 (8)	0.0124 (8)	0.0019 (6)	0.0000 (6)	−0.0010 (6)
C31	0.0197 (9)	0.0235 (9)	0.0177 (8)	0.0093 (7)	0.0036 (7)	0.0068 (7)
C13	0.0230 (9)	0.0199 (9)	0.0206 (9)	0.0049 (7)	−0.0036 (7)	0.0010 (7)
C11	0.0188 (8)	0.0145 (8)	0.0174 (8)	0.0074 (7)	0.0000 (6)	0.0013 (6)
C45	0.0258 (10)	0.0257 (9)	0.0200 (9)	0.0071 (8)	0.0005 (7)	0.0061 (7)
C223	0.0161 (9)	0.0258 (10)	0.0316 (10)	0.0029 (7)	−0.0056 (7)	0.0017 (8)
C32	0.0235 (10)	0.0259 (10)	0.0253 (9)	0.0078 (8)	0.0030 (7)	0.0080 (8)
C55	0.0573 (15)	0.0217 (10)	0.0224 (10)	0.0181 (10)	−0.0103 (9)	0.0000 (8)

C15	0.0453 (13)	0.0347 (11)	0.0169 (9)	0.0114 (10)	−0.0014 (8)	0.0080 (8)
C36	0.0309 (11)	0.0285 (10)	0.0211 (9)	0.0126 (8)	0.0009 (8)	0.0052 (8)
C26	0.0220 (10)	0.0367 (11)	0.0221 (9)	0.0037 (8)	0.0044 (7)	0.0139 (8)
C16	0.0388 (12)	0.0278 (10)	0.0208 (9)	0.0068 (9)	0.0065 (8)	0.0089 (8)
C225	0.0254 (10)	0.0195 (9)	0.0239 (9)	0.0030 (7)	−0.0014 (7)	0.0081 (7)
C17	0.0237 (9)	0.0174 (8)	0.0206 (9)	0.0047 (7)	0.0024 (7)	0.0030 (7)
C43	0.0175 (9)	0.0245 (9)	0.0295 (10)	0.0053 (7)	−0.0023 (7)	0.0027 (8)
C14	0.0347 (11)	0.0263 (10)	0.0192 (9)	0.0106 (9)	−0.0066 (8)	0.0013 (7)
C222	0.0191 (9)	0.0177 (8)	0.0246 (9)	0.0055 (7)	−0.0030 (7)	0.0017 (7)
C54	0.0603 (15)	0.0148 (9)	0.0238 (10)	0.0060 (9)	−0.0147 (10)	0.0038 (7)
C34	0.0384 (13)	0.0561 (14)	0.0294 (11)	0.0215 (11)	0.0171 (9)	0.0204 (10)
C44	0.0251 (10)	0.0265 (10)	0.0231 (9)	0.0085 (8)	−0.0058 (7)	0.0041 (7)
C114	0.0273 (11)	0.0273 (11)	0.0439 (13)	−0.0104 (9)	−0.0058 (9)	0.0073 (9)
C113	0.0337 (12)	0.0208 (10)	0.0336 (11)	−0.0009 (8)	−0.0073 (9)	−0.0011 (8)
C112	0.0239 (10)	0.0199 (9)	0.0225 (9)	0.0024 (7)	−0.0027 (7)	0.0008 (7)
C111	0.0177 (9)	0.0182 (8)	0.0184 (8)	0.0010 (7)	−0.0035 (7)	0.0031 (7)
C35	0.0460 (13)	0.0426 (12)	0.0201 (10)	0.0208 (11)	0.0070 (9)	0.0065 (9)
C115	0.0196 (10)	0.0410 (12)	0.0318 (11)	−0.0038 (9)	0.0011 (8)	0.0102 (9)
C33	0.0259 (11)	0.0371 (12)	0.0389 (12)	0.0068 (9)	0.0074 (9)	0.0180 (9)
C53	0.0406 (12)	0.0219 (10)	0.0263 (10)	−0.0013 (9)	−0.0109 (9)	0.0090 (8)

Geometric parameters (Å, °)

Rh—O1	2.0054 (12)	C52—C51	1.390 (3)
Rh—O2	2.0225 (12)	C52—C53	1.399 (3)
Rh—N2	2.0233 (13)	C52—H52	0.9500
Rh—N1	2.0536 (14)	C221—C222	1.389 (2)
Rh—P	2.2704 (4)	C31—C36	1.397 (3)
Rh—Cl	2.4373 (4)	C31—C32	1.397 (3)
P—C31	1.8175 (18)	C13—C14	1.375 (3)
P—C51	1.8220 (18)	C13—H13	0.9500
P—C41	1.8290 (17)	C11—C17	1.390 (3)
F24—C224	1.358 (2)	C45—C44	1.385 (3)
O2—C21	1.311 (2)	C45—H45	0.9500
O1—C11	1.295 (2)	C223—C222	1.390 (3)
F14—C114	1.359 (2)	C223—H223	0.9500
N1—C12	1.334 (2)	C32—C33	1.388 (3)
N1—C111	1.422 (2)	C32—H32	0.9500
N2—C22	1.325 (2)	C55—C54	1.377 (3)
N2—C221	1.425 (2)	C55—H55	0.9500
C41—C42	1.392 (2)	C15—C16	1.378 (3)
C41—C46	1.396 (3)	C15—C14	1.387 (3)
C21—C27	1.389 (3)	C15—H15	0.9500
C21—C22	1.460 (2)	C36—C35	1.386 (3)
C226—C225	1.390 (3)	C36—H36	0.9500
C226—C221	1.391 (2)	C26—H26	0.9500
C226—H226	0.9500	C16—C17	1.392 (3)
C24—C23	1.371 (3)	C16—H16	0.9500
C24—C25	1.401 (3)	C225—H225	0.9500

C24—H24	0.9500	C17—H17	0.9500
C116—C115	1.387 (3)	C43—C44	1.383 (3)
C116—C111	1.391 (3)	C43—H43	0.9500
C116—H116	0.9500	C14—H14	0.9500
C12—C13	1.425 (2)	C222—H222	0.9500
C12—C11	1.461 (2)	C54—C53	1.381 (3)
C25—C26	1.368 (3)	C54—H54	0.9500
C25—H25	0.9500	C34—C35	1.375 (3)
C46—C45	1.387 (2)	C34—C33	1.387 (3)
C46—H46	0.9500	C34—H34	0.9500
C27—C26	1.402 (3)	C44—H44	0.9500
C27—H27	0.9500	C114—C113	1.368 (3)
C22—C23	1.429 (2)	C114—C115	1.373 (3)
C56—C55	1.389 (3)	C113—C112	1.389 (3)
C56—C51	1.399 (3)	C113—H113	0.9500
C56—H56	0.9500	C112—C111	1.395 (3)
C23—H23	0.9500	C112—H112	0.9500
C42—C43	1.391 (3)	C35—H35	0.9500
C42—H42	0.9500	C115—H115	0.9500
C224—C223	1.372 (3)	C33—H33	0.9500
C224—C225	1.376 (3)	C53—H53	0.9500
O1—Rh—O2	175.41 (5)	C36—C31—P	121.33 (15)
O1—Rh—N2	98.36 (5)	C32—C31—P	119.58 (14)
O2—Rh—N2	78.32 (5)	C14—C13—C12	130.19 (19)
O1—Rh—N1	78.62 (5)	C14—C13—H13	114.9
O2—Rh—N1	104.41 (5)	C12—C13—H13	114.9
N2—Rh—N1	174.43 (5)	O1—C11—C17	117.59 (16)
O1—Rh—P	90.79 (3)	O1—C11—C12	116.25 (15)
O2—Rh—P	92.63 (4)	C17—C11—C12	126.09 (15)
N2—Rh—P	94.69 (4)	C44—C45—C46	120.07 (18)
N1—Rh—P	90.06 (4)	C44—C45—H45	120.0
O1—Rh—Cl	89.39 (3)	C46—C45—H45	120.0
O2—Rh—Cl	87.39 (4)	C224—C223—C222	118.55 (17)
N2—Rh—Cl	89.02 (4)	C224—C223—H223	120.7
N1—Rh—Cl	86.27 (4)	C222—C223—H223	120.7
P—Rh—Cl	176.222 (15)	C33—C32—C31	120.28 (18)
C31—P—C51	106.84 (8)	C33—C32—H32	119.9
C31—P—C41	107.47 (8)	C31—C32—H32	119.9
C51—P—C41	99.36 (8)	C54—C55—C56	120.3 (2)
C31—P—Rh	110.08 (6)	C54—C55—H55	119.8
C51—P—Rh	115.27 (6)	C56—C55—H55	119.8
C41—P—Rh	116.88 (6)	C16—C15—C14	126.52 (19)
C21—O2—Rh	115.43 (11)	C16—C15—H15	116.7
C11—O1—Rh	116.17 (11)	C14—C15—H15	116.7
C12—N1—C111	121.24 (14)	C35—C36—C31	120.2 (2)
C12—N1—Rh	114.11 (11)	C35—C36—H36	119.9
C111—N1—Rh	123.71 (11)	C31—C36—H36	119.9
C22—N2—C221	121.41 (14)	C25—C26—C27	129.62 (18)
C22—N2—Rh	116.04 (11)	C25—C26—H26	115.2

C221—N2—Rh	121.79 (11)	C27—C26—H26	115.2
C42—C41—C46	118.87 (16)	C15—C16—C17	129.42 (19)
C42—C41—P	124.62 (14)	C15—C16—H16	115.3
C46—C41—P	116.38 (13)	C17—C16—H16	115.3
O2—C21—C27	117.17 (16)	C224—C225—C226	118.08 (17)
O2—C21—C22	115.86 (15)	C224—C225—H225	121.0
C27—C21—C22	126.89 (16)	C226—C225—H225	121.0
C225—C226—C221	120.30 (16)	C11—C17—C16	130.78 (18)
C225—C226—H226	119.9	C11—C17—H17	114.6
C221—C226—H226	119.9	C16—C17—H17	114.6
C23—C24—C25	130.34 (18)	C44—C43—C42	120.41 (18)
C23—C24—H24	114.8	C44—C43—H43	119.8
C25—C24—H24	114.8	C42—C43—H43	119.8
C115—C116—C111	119.92 (18)	C13—C14—C15	130.39 (19)
C115—C116—H116	120.0	C13—C14—H14	114.8
C111—C116—H116	120.0	C15—C14—H14	114.8
N1—C12—C13	122.74 (16)	C221—C222—C223	119.97 (17)
N1—C12—C11	113.09 (14)	C221—C222—H222	120.0
C13—C12—C11	123.96 (16)	C223—C222—H222	120.0
C26—C25—C24	126.70 (17)	C55—C54—C53	120.14 (19)
C26—C25—H25	116.6	C55—C54—H54	119.9
C24—C25—H25	116.6	C53—C54—H54	119.9
C45—C46—C41	120.61 (17)	C35—C34—C33	120.3 (2)
C45—C46—H46	119.7	C35—C34—H34	119.8
C41—C46—H46	119.7	C33—C34—H34	119.8
C21—C27—C26	130.54 (18)	C43—C44—C45	119.78 (17)
C21—C27—H27	114.7	C43—C44—H44	120.1
C26—C27—H27	114.7	C45—C44—H44	120.1
N2—C22—C23	122.05 (16)	F14—C114—C113	118.4 (2)
N2—C22—C21	113.11 (15)	F14—C114—C115	118.8 (2)
C23—C22—C21	124.78 (16)	C113—C114—C115	122.80 (19)
C55—C56—C51	120.1 (2)	C114—C113—C112	118.70 (19)
C55—C56—H56	119.9	C114—C113—H113	120.7
C51—C56—H56	119.9	C112—C113—H113	120.7
C24—C23—C22	130.33 (18)	C113—C112—C111	119.88 (19)
C24—C23—H23	114.8	C113—C112—H112	120.1
C22—C23—H23	114.8	C111—C112—H112	120.1
C43—C42—C41	120.25 (17)	C116—C111—C112	119.95 (17)
C43—C42—H42	119.9	C116—C111—N1	118.97 (16)
C41—C42—H42	119.9	C112—C111—N1	120.87 (17)
F24—C224—C223	118.36 (17)	C34—C35—C36	120.3 (2)
F24—C224—C225	118.60 (17)	C34—C35—H35	119.9
C223—C224—C225	123.04 (17)	C36—C35—H35	119.9
C51—C52—C53	119.88 (19)	C114—C115—C116	118.7 (2)
C51—C52—H52	120.1	C114—C115—H115	120.6
C53—C52—H52	120.1	C116—C115—H115	120.6
C52—C51—C56	119.27 (17)	C34—C33—C32	119.8 (2)
C52—C51—P	120.79 (14)	C34—C33—H33	120.1
C56—C51—P	119.46 (15)	C32—C33—H33	120.1

C222—C221—C226	120.02 (16)	C54—C53—C52	120.2 (2)
C222—C221—N2	120.75 (15)	C54—C53—H53	119.9
C226—C221—N2	119.22 (15)	C52—C53—H53	119.9
C36—C31—C32	118.92 (17)		
O1—Rh—P—C31	−10.46 (7)	C41—P—C51—C52	98.78 (15)
O2—Rh—P—C31	172.59 (7)	Rh—P—C51—C52	−26.99 (16)
N2—Rh—P—C31	−108.92 (8)	C31—P—C51—C56	38.42 (16)
N1—Rh—P—C31	68.16 (8)	C41—P—C51—C56	−73.15 (15)
O1—Rh—P—C51	−131.37 (7)	Rh—P—C51—C56	161.08 (12)
O2—Rh—P—C51	51.68 (7)	C225—C226—C221—C222	−2.0 (3)
N2—Rh—P—C51	130.17 (7)	C225—C226—C221—N2	178.53 (16)
N1—Rh—P—C51	−52.75 (7)	C22—N2—C221—C222	74.0 (2)
O1—Rh—P—C41	112.47 (7)	Rh—N2—C221—C222	−116.35 (15)
O2—Rh—P—C41	−64.48 (7)	C22—N2—C221—C226	−106.50 (18)
N2—Rh—P—C41	14.01 (8)	Rh—N2—C221—C226	63.10 (19)
N1—Rh—P—C41	−168.91 (8)	C51—P—C31—C36	25.98 (17)
N2—Rh—O2—C21	7.17 (11)	C41—P—C31—C36	131.85 (15)
N1—Rh—O2—C21	−167.84 (11)	Rh—P—C31—C36	−99.86 (14)
P—Rh—O2—C21	101.42 (11)	C51—P—C31—C32	−158.86 (14)
Cl—Rh—O2—C21	−82.36 (11)	C41—P—C31—C32	−53.00 (16)
N2—Rh—O1—C11	−172.10 (11)	Rh—P—C31—C32	75.29 (15)
N1—Rh—O1—C11	3.14 (11)	N1—C12—C13—C14	−171.02 (18)
P—Rh—O1—C11	93.05 (11)	C11—C12—C13—C14	14.7 (3)
Cl—Rh—O1—C11	−83.18 (11)	Rh—O1—C11—C17	−173.25 (12)
O1—Rh—N1—C12	−10.19 (11)	Rh—O1—C11—C12	3.86 (18)
O2—Rh—N1—C12	166.28 (11)	N1—C12—C11—O1	−12.5 (2)
P—Rh—N1—C12	−100.98 (12)	C13—C12—C11—O1	162.26 (16)
Cl—Rh—N1—C12	79.95 (12)	N1—C12—C11—C17	164.28 (16)
O1—Rh—N1—C111	−179.21 (14)	C13—C12—C11—C17	−20.9 (3)
O2—Rh—N1—C111	−2.74 (14)	C41—C46—C45—C44	−0.9 (3)
P—Rh—N1—C111	90.00 (13)	F24—C224—C223—C222	178.37 (17)
Cl—Rh—N1—C111	−89.08 (13)	C225—C224—C223—C222	−0.8 (3)
O1—Rh—N2—C22	166.48 (12)	C36—C31—C32—C33	−4.3 (3)
O2—Rh—N2—C22	−10.30 (12)	P—C31—C32—C33	−179.58 (15)
P—Rh—N2—C22	−102.03 (12)	C51—C56—C55—C54	−0.7 (3)
Cl—Rh—N2—C22	77.23 (12)	C32—C31—C36—C35	3.7 (3)
O1—Rh—N2—C221	−3.65 (13)	P—C31—C36—C35	178.93 (15)
O2—Rh—N2—C221	179.57 (13)	C24—C25—C26—C27	−1.3 (4)
P—Rh—N2—C221	87.84 (12)	C21—C27—C26—C25	2.1 (4)
Cl—Rh—N2—C221	−92.90 (12)	C14—C15—C16—C17	−1.7 (4)
C31—P—C41—C42	1.24 (17)	F24—C224—C225—C226	−179.86 (16)
C51—P—C41—C42	112.31 (16)	C223—C224—C225—C226	−0.7 (3)
Rh—P—C41—C42	−123.03 (14)	C221—C226—C225—C224	2.1 (3)
C31—P—C41—C46	−174.68 (13)	O1—C11—C17—C16	−172.75 (18)
C51—P—C41—C46	−63.60 (15)	C12—C11—C17—C16	10.5 (3)
Rh—P—C41—C46	61.05 (14)	C15—C16—C17—C11	2.9 (4)
Rh—O2—C21—C27	179.52 (12)	C41—C42—C43—C44	0.0 (3)
Rh—O2—C21—C22	−3.39 (18)	C12—C13—C14—C15	1.2 (4)
C111—N1—C12—C13	9.2 (3)	C16—C15—C14—C13	−6.3 (4)

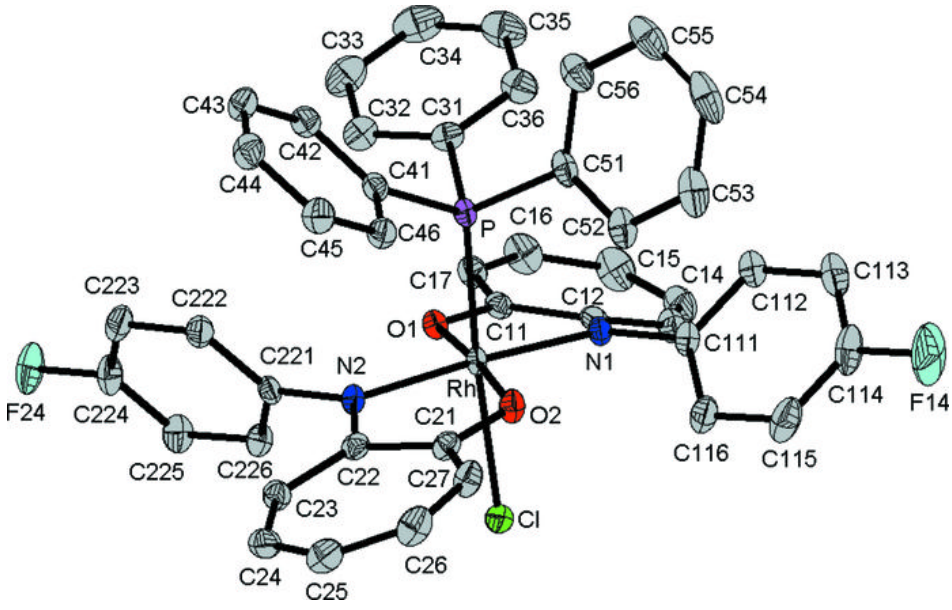
Rh—N1—C12—C13	−160.07 (13)	C226—C221—C222—C223	0.5 (3)
C111—N1—C12—C11	−175.88 (15)	N2—C221—C222—C223	179.92 (16)
Rh—N1—C12—C11	14.80 (18)	C224—C223—C222—C221	0.9 (3)
C23—C24—C25—C26	−4.6 (3)	C56—C55—C54—C53	−0.8 (3)
C42—C41—C46—C45	1.6 (3)	C42—C43—C44—C45	0.7 (3)
P—C41—C46—C45	177.74 (14)	C46—C45—C44—C43	−0.2 (3)
O2—C21—C27—C26	−177.45 (18)	F14—C114—C113—C112	−178.12 (19)
C22—C21—C27—C26	5.8 (3)	C115—C114—C113—C112	0.6 (3)
C221—N2—C22—C23	4.2 (2)	C114—C113—C112—C111	−1.4 (3)
Rh—N2—C22—C23	−166.00 (12)	C115—C116—C111—C112	0.1 (3)
C221—N2—C22—C21	−178.46 (14)	C115—C116—C111—N1	−174.69 (17)
Rh—N2—C22—C21	11.38 (18)	C113—C112—C111—C116	1.1 (3)
O2—C21—C22—N2	−5.2 (2)	C113—C112—C111—N1	175.79 (17)
C27—C21—C22—N2	171.53 (17)	C12—N1—C111—C116	−126.67 (18)
O2—C21—C22—C23	172.07 (15)	Rh—N1—C111—C116	41.6 (2)
C27—C21—C22—C23	−11.2 (3)	C12—N1—C111—C112	58.6 (2)
C25—C24—C23—C22	3.1 (3)	Rh—N1—C111—C112	−133.17 (15)
N2—C22—C23—C24	−176.69 (17)	C33—C34—C35—C36	−1.8 (3)
C21—C22—C23—C24	6.3 (3)	C31—C36—C35—C34	−0.7 (3)
C46—C41—C42—C43	−1.1 (3)	F14—C114—C115—C116	179.30 (19)
P—C41—C42—C43	−176.91 (13)	C113—C114—C115—C116	0.6 (3)
C53—C52—C51—C56	−1.5 (3)	C111—C116—C115—C114	−0.9 (3)
C53—C52—C51—P	−173.49 (14)	C35—C34—C33—C32	1.2 (3)
C55—C56—C51—C52	1.9 (3)	C31—C32—C33—C34	1.9 (3)
C55—C56—C51—P	173.95 (14)	C55—C54—C53—C52	1.1 (3)
C31—P—C51—C52	−149.65 (14)	C51—C52—C53—C54	0.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C116—H116···Cl	0.95	2.83	3.579 (2)	137
C17—H17···F14^{i}	0.95	2.39	3.325 (2)	167
C27—H27···F24^{ii}	0.95	2.63	3.541 (2)	162

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

Fig. 1


C33
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