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Bis(acetonitrile-κN)(η^5-pentamethylcyclopentadienyl)(pyrimidine-κN)-rhodium(III) bis(hexafluoridophosphate)

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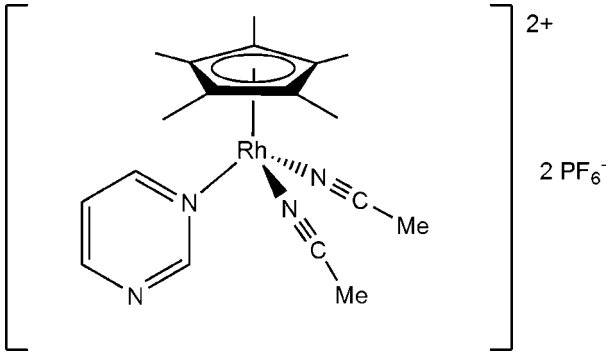
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.004 Å; disorder in solvent or counterion; R factor = 0.037; wR factor = 0.100; data-to-parameter ratio = 16.6.

The title compound, $[Rh(C_{10}H_{15})(C_4H_4N_2)(C_2H_3N)_2](PF_6)_2$ or $[Cp^*Rh(NCMe)_2(N_2C_4H_4)](PF_6)_2$, where Cp* is pentamethylcyclopentadienyl, was obtained from the treatment of an acetonitrile solution of $[Cp^*Rh(NCMe)_3](PF_6)_2$ with an excess of pyrimidine. The Rh^{III} center is coordinated by one Cp* ring, two acetonitrile ligands and one pyrimidine ligand in a pseudo-octahedral geometry. Both PF_6 anions are disordered (site occupancies *ca* 0.4:0.6, and 0.3:0.4:0.3).

Related literature

For selected literature on metal–pyrimidine complexes, see: Barnett *et al.* (2005); Nedelec & Rochon (2001); Sharma *et al.* (1998). For the synthesis of $[Cp^*Rh(NCMe)_3](PF_6)_2$, see: White *et al.* (1992).



Experimental

Crystal data

$[Rh(C_{10}H_{15})(C_4H_4N_2)(C_2H_3N)_2](PF_6)_2$
M_r = 690.27
Orthorhombic, *Pbca*
a = 14.4046 (8) Å
b = 14.7669 (7) Å
c = 24.3537 (13) Å
V = 5180.3 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.89 mm^{-1}
T = 193 (2) K
0.36 × 0.36 × 0.32 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: integration (*SHELXTL* and *XPREP*; Bruker, 2005)
T_{min} = 0.625, T_{max} = 0.813
93720 measured reflections
7612 independent reflections
6384 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.04
7612 reflections
459 parameters
241 restraints
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}

Table 1
Selected bond lengths (Å).

Rh1—N1	2.093 (2)	Rh1—N3	2.148 (2)
Rh1—N2	2.110 (2)	Rh1—C2	2.149 (2)
Rh1—C4	2.136 (3)	Rh1—C3	2.156 (3)
Rh1—C1	2.140 (2)	Rh1—C5	2.176 (3)

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2005); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *XCIF* (Bruker, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2063).

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supplementary materials

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Bis(acetonitrile-κN)(η^5-pentamethylcyclopentadienyl)(pyrimidine-κN)rhodium(III) bis(hexafluoridophosphate)

J. L. Boyer, S. R. Wilson and T. B. Rauchfuss

Comment

While pyrimidine and pyrimidine derivatives are biologically relevant, only 120 crystal structures with metal–pyrimidine bonds have been reported, none of which contain Cp co-ligands (Barnett *et al.*, 2005; Nedelec & Rochon, 2001; and Sharma *et al.*, 1998). Here we report the crystal structure of $[Cp^*Rh(NCMe)_2(N_2C_4H_4)](PF_6)_2$ as an unique half-sandwich pyrimidine adduct. The Rh—N distance for the two acetonitrile ligands are 2.093 (2) and 2.109 (2) Å. The coordinated pyrimidine has a longer Rh—N distance of 2.148 (2) Å. The N—Rh—N angles are slightly contracted ranging from 86.05 (9) to 88.74 (10)°.

Experimental

$[Cp^*Rh(NCMe)_3](PF_6)_2$ was prepared according to literature methods (White *et al.*, 1992). The compound was synthesized by dissolving 95 mg (0.15 mmol) $[Cp^*Rh(NCMe)_3](PF_6)_2$ and 35 mg (0.44 mmol) pyrimidine in 2 ml MeCN. Yellow crystals were grown at room temperature by vapor diffusion of diethylether into an acetonitrile solution.

Refinement

The proposed model includes multiple disordered sites for the two anions. Disordered anion moieties were refined as rigid, idealized groups with similar amplitude restraints imposed on displacement parameters for overlapping sites separated by less than Van der Waals radii using an effective standard deviation of 0.01 Å. The single idealized group refinement for the first set converged with some principal mean square atomic displacements that differed by as much as a factor of ten and some that were nearly isotropic. This suggested that a single rigid body with anisotropic displacement parameters was a poor fit to the observed data. In addition, residual electron density in excess of 2 e/Å^3 from a subsequent difference Fourier map clearly indicated multiple potential surfaces for this anion. After refining two rigid groups (P1, P3) for the first set, residual density from a subsequent difference Fourier map indicated reasonable atomic positions for a third group. The proposed model for the second anion set (P2, P4) was developed simultaneously in a like manner. Methyl H atom positions, R—CH_3, were optimized by rotation about R—C bonds with idealized C—H, R—H and H···H distances. Remaining H atoms were included as riding idealized contributors. Methyl H atom U's were assigned as 1.5 times U_{eq} of the carrier atom; remaining H atom U's were assigned as 1.2 times the carrier U_{eq}.

Figures

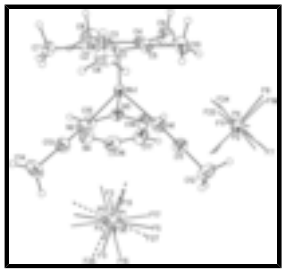


Fig. 1. *SHELXTL/XP* (Bruker, 2005) plot showing 50% probability ellipsoids for non-H atoms and circles of arbitrary size for H atoms. Disordered anions were draw schematically with minimal labels for clarity.

Bis(acetonitrile-κ*N*)(η^5-pentamethylcyclopentadienyl)(pyrimidine- κ*N*)rhodium(III) bis(hexafluoridophosphate)

Crystal data

$[Rh(C_{10}H_{15})(C_4H_4N_2)(C_2H_3N)_2](PF_6)_2$	F_{000} = 2752
M_r = 690.27	D_x = 1.770 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 9298 reflections
a = 14.4046 (8) Å	θ = 2.2–30.7º
b = 14.7669 (7) Å	μ = 0.89 mm^{-1}
c = 24.3537 (13) Å	*T* = 193 (2) K
V = 5180.3 (5) Å^3	Prism, yellow
Z = 8	0.36 × 0.36 × 0.32 mm

Data collection

Bruker Kappa APEXII CCD diffractometer	7612 independent reflections
Radiation source: fine-focus sealed tube	6384 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 193(2) K	θ_{max} = 30.1º
profile data from φ and ω scans	θ_{min} = 1.7º
Absorption correction: integration (SHELXTL and XPREP; Bruker, 2005)	*h* = −20→19
T_{min} = 0.625, T_{max} = 0.813	*k* = −20→20
93720 measured reflections	*l* = −34→34

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H-atom parameters not refined
$wR(F^2)$ = 0.100	$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 9.0148P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.017

7612 reflections	$\Delta\rho_{max}$ = 0.93 e Å^{-3}
459 parameters	$\Delta\rho_{min}$ = −0.72 e Å^{-3}
241 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. One distinct cell was identified using *APEX2* (Bruker, 2004). Five frame series were integrated and filtered for statistical outliers using *SAINT* (Bruker, 2005) then corrected for absorption by integration using *SHELXTL*/*XPREP* (Bruker, 2005) before using *SAINT*/*SADABS* (Bruker, 2005) to sort, merge, and scale the combined data. No decay correction was applied.

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. Structure was phased by direct methods. Systematic conditions suggested the unambiguous space group. The space group choice was confirmed by successful convergence of the full-matrix least-squares refinement on F^2. The highest peaks in the final difference Fourier map were in the vicinity of atoms F7 and F3; the final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed no dependence on amplitude or resolution.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Rh1	0.568281 (13)	0.322308 (12)	0.639265 (8)	0.02201 (6)	
C1	0.59292 (19)	0.43808 (17)	0.69007 (11)	0.0269 (5)	
C2	0.68007 (17)	0.39330 (16)	0.67877 (10)	0.0239 (5)	
C3	0.67538 (19)	0.30338 (17)	0.70001 (11)	0.0275 (5)	
C4	0.5845 (2)	0.2917 (2)	0.72445 (11)	0.0318 (6)	
C5	0.53674 (19)	0.3764 (2)	0.72025 (11)	0.0315 (5)	
C6	0.5700 (3)	0.5338 (2)	0.67585 (15)	0.0435 (7)	
H6A	0.5898	0.5737	0.7057	0.065*	
H6B	0.5028	0.5396	0.6705	0.065*	
H6C	0.6022	0.5508	0.6419	0.065*	
C7	0.7606 (2)	0.4361 (2)	0.65047 (12)	0.0353 (6)	
H7A	0.7996	0.4672	0.6775	0.053*	
H7B	0.7381	0.4799	0.6234	0.053*	
H7C	0.7972	0.3893	0.6319	0.053*	
C8	0.7502 (2)	0.2337 (2)	0.69899 (14)	0.0441 (7)	
H8A	0.7795	0.2301	0.7353	0.066*	
H8B	0.7969	0.2505	0.6716	0.066*	
H8C	0.7235	0.1747	0.6895	0.066*	
C9	0.5515 (3)	0.2092 (3)	0.75445 (17)	0.0576 (10)	
H9A	0.5662	0.2151	0.7936	0.086*	
H9B	0.5826	0.1555	0.7396	0.086*	
H9C	0.4843	0.2030	0.7498	0.086*	
C10	0.4433 (2)	0.3962 (3)	0.74368 (15)	0.0548 (10)	
H10A	0.4492	0.4088	0.7830	0.082*	

H10B	0.4026	0.3438	0.7383	0.082*	
H10C	0.4167	0.4491	0.7251	0.082*	
N1	0.42867 (16)	0.31056 (16)	0.61660 (11)	0.0320 (5)	
C11	0.3546 (2)	0.30076 (18)	0.60177 (12)	0.0319 (5)	
C12	0.2609 (2)	0.2874 (2)	0.58173 (15)	0.0462 (8)	
H12A	0.2424	0.3395	0.5593	0.069*	
H12B	0.2184	0.2814	0.6129	0.069*	
H12C	0.2585	0.2322	0.5594	0.069*	
C13	0.6125 (2)	0.42360 (19)	0.52430 (11)	0.0337 (6)	
N2	0.59482 (18)	0.38485 (16)	0.56298 (9)	0.0317 (5)	
C14	0.6351 (3)	0.4750 (3)	0.47474 (13)	0.0520 (9)	
H14A	0.6240	0.5396	0.4813	0.078*	
H14B	0.5958	0.4543	0.4444	0.078*	
H14C	0.7005	0.4656	0.4653	0.078*	
N3	0.58730 (16)	0.19358 (15)	0.59979 (10)	0.0280 (4)	
C15	0.6593 (2)	0.17756 (19)	0.56566 (12)	0.0345 (6)	
H15	0.7032	0.2250	0.5610	0.041*	
N4	0.67417 (19)	0.10158 (18)	0.53820 (11)	0.0402 (6)	
C16	0.6122 (2)	0.0354 (2)	0.54516 (14)	0.0408 (7)	
H16	0.6202	−0.0196	0.5255	0.049*	
C17	0.5376 (2)	0.0438 (2)	0.57957 (15)	0.0415 (7)	
H17	0.4949	−0.0045	0.5847	0.050*	
C18	0.5271 (2)	0.12540 (19)	0.60656 (13)	0.0353 (6)	
H18	0.4758	0.1334	0.6306	0.042*	
P1	0.4462 (3)	0.2436 (2)	0.43923 (14)	0.0403 (15)	0.408 (5)
F1	0.3842 (4)	0.3239 (3)	0.4127 (3)	0.081 (2)	0.408 (5)
F2	0.5083 (4)	0.1632 (3)	0.4658 (3)	0.090 (2)	0.408 (5)
F3	0.4497 (4)	0.1931 (4)	0.38019 (18)	0.072 (2)	0.408 (5)
F4	0.4428 (5)	0.2940 (4)	0.49825 (19)	0.076 (2)	0.408 (5)
F5	0.3525 (3)	0.1885 (3)	0.4546 (2)	0.0509 (17)	0.408 (5)
F6	0.5400 (3)	0.2986 (4)	0.4238 (3)	0.078 (2)	0.408 (5)
P2	0.28776 (14)	0.02841 (15)	0.67394 (8)	0.0362 (6)	0.588 (5)
F7	0.18034 (15)	0.0385 (4)	0.65521 (14)	0.0862 (18)	0.588 (5)
F8	0.39517 (16)	0.0183 (3)	0.69267 (14)	0.0647 (14)	0.588 (5)
F9	0.2574 (3)	0.0414 (2)	0.73750 (9)	0.0506 (13)	0.588 (5)
F10	0.3182 (2)	0.0155 (3)	0.61038 (9)	0.0713 (17)	0.588 (5)
F11	0.3014 (3)	0.13688 (15)	0.66808 (17)	0.0900 (18)	0.588 (5)
F12	0.2742 (3)	−0.08006 (16)	0.67979 (17)	0.0821 (15)	0.588 (5)
P3	0.4535 (4)	0.2487 (3)	0.43830 (17)	0.034 (3)	0.304 (4)
F13	0.4356 (6)	0.3326 (5)	0.4798 (3)	0.061 (2)	0.304 (4)
F14	0.4713 (6)	0.1648 (4)	0.3967 (3)	0.055 (2)	0.304 (4)
F15	0.3741 (5)	0.2876 (5)	0.3975 (3)	0.077 (2)	0.304 (4)
F16	0.5329 (5)	0.2098 (6)	0.4791 (3)	0.099 (3)	0.304 (4)
F17	0.3759 (5)	0.1897 (5)	0.4705 (3)	0.080 (3)	0.304 (4)
F18	0.5311 (5)	0.3078 (5)	0.4061 (3)	0.083 (3)	0.304 (4)
P4	0.2829 (2)	0.04411 (19)	0.66883 (12)	0.0334 (7)	0.412 (5)
F19	0.2476 (4)	0.0260 (3)	0.73103 (13)	0.0478 (17)	0.412 (5)
F20	0.3182 (3)	0.0622 (3)	0.60663 (13)	0.0514 (16)	0.412 (5)
F21	0.1967 (3)	0.1128 (4)	0.6591 (2)	0.087 (2)	0.412 (5)

F22	0.3690 (4)	−0.0246 (4)	0.6786 (2)	0.090 (2)	0.412 (5)
F23	0.2198 (4)	−0.0395 (4)	0.6474 (2)	0.088 (2)	0.412 (5)
F24	0.3460 (4)	0.1277 (3)	0.6903 (2)	0.079 (2)	0.412 (5)
P5	0.4569 (3)	0.2483 (3)	0.44008 (16)	0.028 (2)	0.288 (4)
F25	0.4469 (6)	0.2722 (6)	0.37544 (17)	0.085 (2)	0.288 (4)
F26	0.4668 (6)	0.2243 (6)	0.50474 (18)	0.094 (2)	0.288 (4)
F27	0.3520 (4)	0.2086 (5)	0.4403 (3)	0.057 (2)	0.288 (4)
F28	0.5617 (4)	0.2879 (6)	0.4399 (4)	0.090 (3)	0.288 (4)
F29	0.4174 (6)	0.3477 (4)	0.4557 (4)	0.077 (3)	0.288 (4)
F30	0.4963 (6)	0.1488 (4)	0.4244 (4)	0.082 (2)	0.288 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rh1	0.02173 (10)	0.02244 (10)	0.02185 (10)	−0.00308 (7)	−0.00013 (7)	0.00192 (6)
C1	0.0279 (12)	0.0266 (11)	0.0262 (12)	0.0018 (9)	−0.0002 (10)	−0.0038 (9)
C2	0.0234 (11)	0.0271 (11)	0.0212 (10)	−0.0023 (9)	−0.0004 (9)	−0.0015 (9)
C3	0.0292 (13)	0.0275 (11)	0.0259 (12)	0.0013 (9)	−0.0046 (10)	0.0012 (9)
C4	0.0334 (14)	0.0382 (14)	0.0237 (12)	−0.0083 (11)	−0.0022 (10)	0.0078 (10)
C5	0.0244 (12)	0.0458 (15)	0.0242 (12)	−0.0021 (11)	0.0030 (10)	−0.0020 (11)
C6	0.054 (2)	0.0292 (14)	0.0475 (18)	0.0098 (13)	−0.0076 (15)	−0.0049 (13)
C7	0.0292 (14)	0.0434 (15)	0.0332 (14)	−0.0106 (12)	0.0028 (11)	−0.0006 (11)
C8	0.0438 (17)	0.0386 (15)	0.0498 (18)	0.0137 (13)	−0.0116 (15)	−0.0009 (13)
C9	0.068 (2)	0.058 (2)	0.047 (2)	−0.0242 (19)	−0.0037 (18)	0.0267 (18)
C10	0.0317 (16)	0.091 (3)	0.0420 (18)	0.0036 (17)	0.0129 (14)	−0.0070 (19)
N1	0.0289 (12)	0.0328 (11)	0.0342 (12)	−0.0012 (9)	−0.0028 (9)	0.0024 (9)
C11	0.0314 (14)	0.0301 (12)	0.0343 (14)	−0.0025 (10)	−0.0041 (11)	0.0027 (10)
C12	0.0342 (16)	0.0484 (17)	0.056 (2)	−0.0040 (14)	−0.0166 (15)	0.0043 (15)
C13	0.0392 (15)	0.0328 (13)	0.0290 (13)	−0.0071 (11)	−0.0004 (11)	−0.0003 (10)
N2	0.0364 (12)	0.0327 (11)	0.0260 (11)	−0.0072 (10)	−0.0013 (9)	0.0011 (9)
C14	0.071 (2)	0.0529 (19)	0.0322 (16)	−0.0148 (18)	0.0076 (16)	0.0122 (14)
N3	0.0289 (11)	0.0249 (9)	0.0302 (11)	−0.0024 (8)	−0.0014 (9)	−0.0007 (8)
C15	0.0324 (14)	0.0336 (13)	0.0376 (15)	−0.0033 (11)	0.0032 (12)	−0.0026 (11)
N4	0.0398 (14)	0.0374 (13)	0.0434 (14)	0.0025 (11)	0.0020 (11)	−0.0061 (11)
C16	0.0440 (17)	0.0309 (13)	0.0475 (18)	0.0039 (12)	−0.0075 (14)	−0.0073 (12)
C17	0.0397 (16)	0.0274 (13)	0.057 (2)	−0.0057 (12)	−0.0040 (15)	−0.0009 (13)
C18	0.0339 (14)	0.0285 (12)	0.0435 (16)	−0.0052 (11)	0.0011 (12)	0.0020 (11)
P1	0.048 (3)	0.036 (2)	0.037 (3)	−0.0051 (19)	−0.012 (2)	−0.0006 (19)
F1	0.085 (4)	0.055 (4)	0.103 (5)	0.004 (3)	−0.015 (4)	0.031 (4)
F2	0.092 (4)	0.069 (4)	0.108 (5)	0.019 (3)	−0.065 (4)	0.008 (4)
F3	0.078 (4)	0.085 (5)	0.053 (4)	0.003 (4)	0.001 (3)	−0.022 (4)
F4	0.096 (4)	0.084 (5)	0.047 (4)	−0.017 (4)	−0.004 (3)	−0.027 (3)
F5	0.056 (3)	0.050 (3)	0.046 (4)	−0.019 (3)	−0.010 (3)	0.015 (3)
F6	0.042 (3)	0.077 (4)	0.116 (6)	−0.037 (3)	0.013 (4)	−0.015 (4)
P2	0.0333 (11)	0.0463 (10)	0.0290 (9)	−0.0026 (8)	−0.0009 (7)	0.0082 (8)
F7	0.038 (2)	0.173 (5)	0.048 (2)	0.005 (3)	−0.0042 (17)	0.030 (3)
F8	0.0369 (19)	0.106 (4)	0.051 (2)	−0.013 (2)	−0.0052 (17)	0.023 (2)
F9	0.064 (3)	0.049 (2)	0.038 (2)	−0.006 (2)	0.005 (2)	0.0008 (18)

F10	0.054 (2)	0.130 (5)	0.0303 (19)	−0.007 (3)	0.0069 (17)	0.004 (2)
F11	0.136 (5)	0.051 (2)	0.083 (4)	0.003 (3)	0.022 (3)	0.032 (2)
F12	0.101 (4)	0.059 (2)	0.087 (3)	−0.018 (2)	0.021 (3)	−0.020 (2)
P3	0.035 (4)	0.032 (4)	0.036 (4)	−0.011 (3)	−0.003 (4)	−0.005 (3)
F13	0.081 (5)	0.062 (5)	0.040 (5)	0.012 (4)	−0.014 (4)	−0.021 (4)
F14	0.084 (6)	0.026 (3)	0.056 (5)	0.008 (3)	−0.007 (4)	−0.012 (3)
F15	0.082 (5)	0.064 (5)	0.085 (5)	0.007 (4)	−0.037 (4)	0.014 (4)
F16	0.102 (5)	0.098 (5)	0.098 (5)	0.031 (5)	−0.041 (4)	0.000 (5)
F17	0.077 (5)	0.083 (5)	0.078 (6)	−0.022 (4)	0.000 (5)	0.012 (4)
F18	0.075 (5)	0.073 (5)	0.101 (6)	−0.009 (4)	0.008 (5)	0.004 (5)
P4	0.0357 (15)	0.0394 (12)	0.0251 (13)	−0.0036 (10)	−0.0032 (10)	0.0008 (10)
F19	0.059 (4)	0.064 (4)	0.020 (2)	−0.018 (3)	−0.002 (2)	0.000 (2)
F20	0.044 (3)	0.079 (4)	0.032 (3)	−0.009 (3)	0.004 (2)	−0.006 (3)
F21	0.071 (4)	0.116 (5)	0.074 (4)	0.032 (4)	0.023 (3)	0.032 (4)
F22	0.080 (5)	0.119 (5)	0.070 (4)	0.050 (4)	−0.006 (4)	0.010 (4)
F23	0.109 (5)	0.094 (4)	0.062 (4)	−0.064 (4)	0.012 (4)	−0.014 (3)
F24	0.093 (5)	0.088 (5)	0.056 (4)	−0.055 (4)	0.026 (4)	−0.020 (3)
P5	0.031 (3)	0.025 (3)	0.028 (3)	0.008 (3)	−0.009 (3)	−0.005 (3)
F25	0.096 (5)	0.092 (5)	0.068 (4)	0.002 (5)	−0.004 (4)	0.023 (4)
F26	0.099 (5)	0.113 (5)	0.070 (4)	0.010 (5)	−0.031 (4)	0.012 (4)
F27	0.044 (4)	0.067 (5)	0.060 (5)	−0.018 (4)	−0.005 (3)	0.000 (4)
F28	0.059 (5)	0.098 (5)	0.112 (7)	−0.007 (5)	0.001 (5)	−0.029 (5)
F29	0.092 (5)	0.060 (4)	0.078 (6)	0.020 (4)	0.000 (5)	−0.023 (5)
F30	0.101 (5)	0.052 (4)	0.092 (5)	0.020 (4)	−0.007 (5)	−0.004 (4)

Geometric parameters (Å, °)

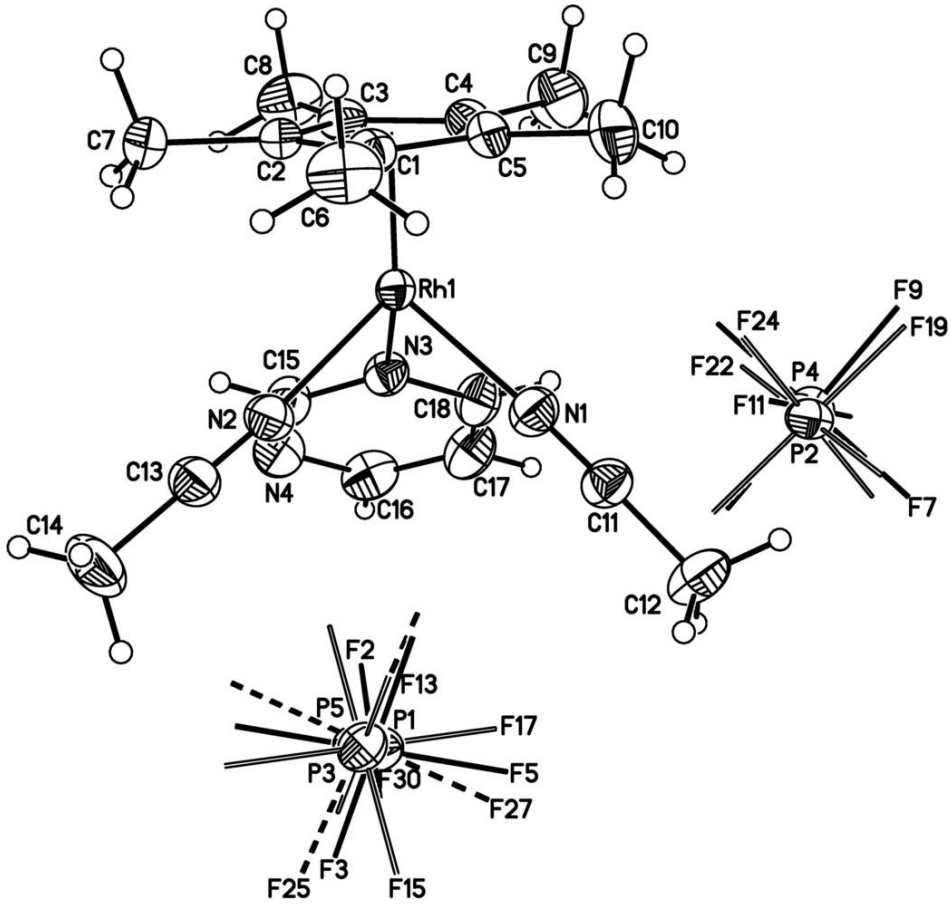
Rh1—N1	2.093 (2)	C14—H14C	0.9800
Rh1—N2	2.110 (2)	N3—C18	1.339 (3)
Rh1—C4	2.136 (3)	N3—C15	1.350 (4)
Rh1—C1	2.140 (2)	C15—N4	1.324 (4)
Rh1—N3	2.148 (2)	C15—H15	0.9500
Rh1—C2	2.149 (2)	N4—C16	1.335 (4)
Rh1—C3	2.156 (3)	C16—C17	1.368 (5)
Rh1—C5	2.176 (3)	C16—H16	0.9500
C1—C5	1.423 (4)	C17—C18	1.381 (4)
C1—C2	1.445 (4)	C17—H17	0.9500
C1—C6	1.492 (4)	C18—H18	0.9500
C2—C3	1.427 (3)	P1—F4	1.6199
C2—C7	1.490 (4)	P1—F6	1.6199
C3—C4	1.448 (4)	P1—F5	1.6200
C3—C8	1.491 (4)	P1—F1	1.6201
C4—C5	1.432 (4)	P1—F3	1.6201
C4—C9	1.498 (4)	P1—F2	1.6202
C5—C10	1.491 (4)	P2—F10	1.6198
C6—H6A	0.9800	P2—F7	1.6199
C6—H6B	0.9800	P2—F8	1.6200
C6—H6C	0.9800	P2—F12	1.6200
C7—H7A	0.9800	P2—F11	1.6200

C7—H7B	0.9800	P2—F9	1.6200
C7—H7C	0.9800	P3—F16	1.6199
C8—H8A	0.9800	P3—F13	1.6199
C8—H8B	0.9800	P3—F18	1.6200
C8—H8C	0.9800	P3—F17	1.6201
C9—H9A	0.9800	P3—F14	1.6201
C9—H9B	0.9800	P3—F15	1.6202
C9—H9C	0.9800	P4—F23	1.6199
C10—H10A	0.9800	P4—F21	1.6200
C10—H10B	0.9800	P4—F22	1.6200
C10—H10C	0.9800	P4—F20	1.6200
N1—C11	1.136 (4)	P4—F19	1.6200
C11—C12	1.449 (4)	P4—F24	1.6201
C12—H12A	0.9800	P5—F25	1.6198
C12—H12B	0.9800	P5—F27	1.6198
C12—H12C	0.9800	P5—F30	1.6199
C13—N2	1.131 (4)	P5—F28	1.6200
C13—C14	1.462 (4)	P5—F29	1.6201
C14—H14A	0.9800	P5—F26	1.6202
C14—H14B	0.9800		
N1—Rh1—N2	88.75 (10)	C13—C14—H14A	109.5
N1—Rh1—C4	110.11 (10)	C13—C14—H14B	109.5
N2—Rh1—C4	158.14 (10)	H14A—C14—H14B	109.5
N1—Rh1—C1	112.22 (10)	C13—C14—H14C	109.5
N2—Rh1—C1	97.43 (9)	H14A—C14—H14C	109.5
C4—Rh1—C1	65.76 (11)	H14B—C14—H14C	109.5
N1—Rh1—N3	86.05 (9)	C18—N3—C15	116.2 (2)
N2—Rh1—N3	88.29 (9)	C18—N3—Rh1	121.9 (2)
C4—Rh1—N3	103.49 (10)	C15—N3—Rh1	121.91 (18)
C1—Rh1—N3	160.86 (10)	N4—C15—N3	125.7 (3)
N1—Rh1—C2	151.48 (10)	N4—C15—H15	117.1
N2—Rh1—C2	92.57 (9)	N3—C15—H15	117.1
C4—Rh1—C2	65.57 (10)	C15—N4—C16	116.7 (3)
C1—Rh1—C2	39.38 (10)	N4—C16—C17	122.5 (3)
N3—Rh1—C2	122.45 (9)	N4—C16—H16	118.8
N1—Rh1—C3	149.10 (10)	C17—C16—H16	118.8
N2—Rh1—C3	122.10 (10)	C16—C17—C18	117.2 (3)
C4—Rh1—C3	39.44 (10)	C16—C17—H17	121.4
C1—Rh1—C3	65.67 (10)	C18—C17—H17	121.4
N3—Rh1—C3	95.81 (9)	N3—C18—C17	121.8 (3)
C2—Rh1—C3	38.71 (9)	N3—C18—H18	119.1
N1—Rh1—C5	93.95 (10)	C17—C18—H18	119.1
N2—Rh1—C5	132.47 (11)	F4—P1—F6	90.0
C4—Rh1—C5	38.77 (11)	F4—P1—F5	90.0
C1—Rh1—C5	38.48 (10)	F6—P1—F5	180.0
N3—Rh1—C5	139.24 (10)	F4—P1—F1	90.0
C2—Rh1—C5	64.63 (10)	F6—P1—F1	90.0
C3—Rh1—C5	64.85 (10)	F5—P1—F1	90.0
C5—C1—C2	107.4 (2)	F4—P1—F3	180.0

C5—C1—C6	126.9 (3)	F6—P1—F3	90.0
C2—C1—C6	125.6 (3)	F5—P1—F3	90.0
C5—C1—Rh1	72.13 (15)	F1—P1—F3	90.0
C2—C1—Rh1	70.64 (14)	F4—P1—F2	90.0
C6—C1—Rh1	125.8 (2)	F6—P1—F2	90.0
C3—C2—C1	108.4 (2)	F5—P1—F2	90.0
C3—C2—C7	126.8 (2)	F1—P1—F2	180.0
C1—C2—C7	124.8 (2)	F3—P1—F2	90.0
C3—C2—Rh1	70.90 (14)	F10—P2—F7	90.0
C1—C2—Rh1	69.98 (14)	F10—P2—F8	90.0
C7—C2—Rh1	125.68 (18)	F7—P2—F8	180.0
C2—C3—C4	107.6 (2)	F10—P2—F12	90.0
C2—C3—C8	127.0 (3)	F7—P2—F12	90.0
C4—C3—C8	125.3 (3)	F8—P2—F12	90.0
C2—C3—Rh1	70.39 (14)	F10—P2—F11	90.0
C4—C3—Rh1	69.56 (15)	F7—P2—F11	90.0
C8—C3—Rh1	126.6 (2)	F8—P2—F11	90.0
C5—C4—C3	107.5 (2)	F12—P2—F11	180.0
C5—C4—C9	126.4 (3)	F10—P2—F9	180.0
C3—C4—C9	125.7 (3)	F7—P2—F9	90.0
C5—C4—Rh1	72.12 (15)	F8—P2—F9	90.0
C3—C4—Rh1	71.00 (15)	F12—P2—F9	90.0
C9—C4—Rh1	127.7 (2)	F11—P2—F9	90.0
C1—C5—C4	108.8 (2)	F16—P3—F13	90.0
C1—C5—C10	125.9 (3)	F16—P3—F18	90.0
C4—C5—C10	125.3 (3)	F13—P3—F18	90.0
C1—C5—Rh1	69.39 (14)	F16—P3—F17	90.0
C4—C5—Rh1	69.11 (15)	F13—P3—F17	90.0
C10—C5—Rh1	127.4 (2)	F18—P3—F17	180.0
C1—C6—H6A	109.5	F16—P3—F14	90.0
C1—C6—H6B	109.5	F13—P3—F14	180.0
H6A—C6—H6B	109.5	F18—P3—F14	90.0
C1—C6—H6C	109.5	F17—P3—F14	90.0
H6A—C6—H6C	109.5	F16—P3—F15	180.0
H6B—C6—H6C	109.5	F13—P3—F15	90.0
C2—C7—H7A	109.5	F18—P3—F15	90.0
C2—C7—H7B	109.5	F17—P3—F15	90.0
H7A—C7—H7B	109.5	F14—P3—F15	90.0
C2—C7—H7C	109.5	F23—P4—F21	90.0
H7A—C7—H7C	109.5	F23—P4—F22	90.0
H7B—C7—H7C	109.5	F21—P4—F22	180.0
C3—C8—H8A	109.5	F23—P4—F20	90.0
C3—C8—H8B	109.5	F21—P4—F20	90.0
H8A—C8—H8B	109.5	F22—P4—F20	90.0
C3—C8—H8C	109.5	F23—P4—F19	90.0
H8A—C8—H8C	109.5	F21—P4—F19	90.0
H8B—C8—H8C	109.5	F22—P4—F19	90.0
C4—C9—H9A	109.5	F20—P4—F19	180.0
C4—C9—H9B	109.5	F23—P4—F24	180.0

H9A—C9—H9B	109.5	F21—P4—F24	90.0
C4—C9—H9C	109.5	F22—P4—F24	90.0
H9A—C9—H9C	109.5	F20—P4—F24	90.0
H9B—C9—H9C	109.5	F19—P4—F24	90.0
C5—C10—H10A	109.5	F25—P5—F27	90.0
C5—C10—H10B	109.5	F25—P5—F30	90.0
H10A—C10—H10B	109.5	F27—P5—F30	90.0
C5—C10—H10C	109.5	F25—P5—F28	90.0
H10A—C10—H10C	109.5	F27—P5—F28	180.0
H10B—C10—H10C	109.5	F30—P5—F28	90.0
C11—N1—Rh1	175.8 (3)	F25—P5—F29	90.0
N1—C11—C12	178.7 (4)	F27—P5—F29	90.0
C11—C12—H12A	109.5	F30—P5—F29	180.0
C11—C12—H12B	109.5	F28—P5—F29	90.0
H12A—C12—H12B	109.5	F25—P5—F26	180.0
C11—C12—H12C	109.5	F27—P5—F26	90.0
H12A—C12—H12C	109.5	F30—P5—F26	90.0
H12B—C12—H12C	109.5	F28—P5—F26	90.0
N2—C13—C14	179.1 (3)	F29—P5—F26	90.0
C13—N2—Rh1	174.6 (2)		

Fig. 1


C8
C9
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F22
P4
N2
C18
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F11
C13
N4
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P2
F7
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