IUCrData

ISSN 2414-3146

(η^4-1,5-Cyclooctadiene)[(*R*)-(+)-5,5′,6,6′,7,7′,8,8′-octahydro-2,2′-bis(diphenylphosphanyl)-1,1′-binaphthyl-κ^2P,P']rhodium(I) tetrafluoroborate 0.72-pentane 0.56-methanol solvate

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Received 18 July 2017
Accepted 28 August 2017

Edited by S. Parkin, University of Kentucky, USA

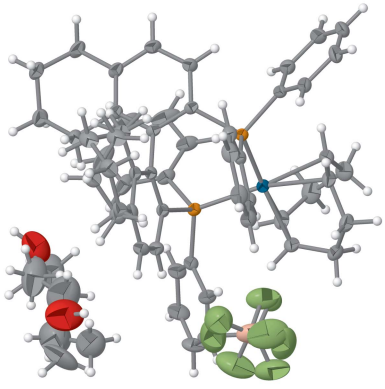
Keywords: crystal structure; rhodium complex; hydrogenation.

CCDC reference: 1531751

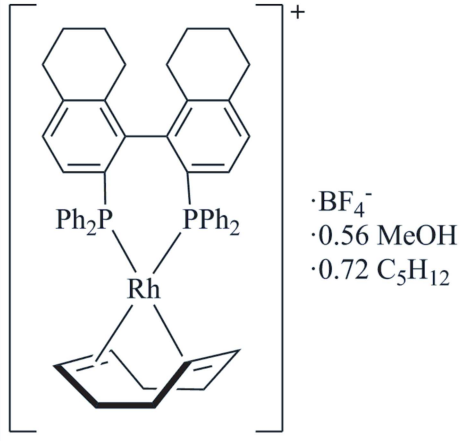
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Rh(C_8H_{12})(C_{44}H_{20}P_2)]BF_4{\cdot}0.72C_5H_{12}{\cdot}0.56{\cdot}CH_4O$, crystallizes in the Sohncke space group $P2_1$. The Rh^I centre is coordinated by a H_8-BINAP 5,5′,6,6′,7,7′,8,8′-octahydro-2,2′-bis(diphenylphosphanyl)-1,1′-binaphthyl ligand and by a bidentate η^2,η^2-coordinated cod (cycloocta-1,5-diene) ligand. The asymmetric unit contains one cation, one anion and cocrystallized pentane [occupancy 0.720 (4)] and methanol [2 × 0.280 (4) occupancy] molecules. The rhodium(I) complex $[Rh(H_8\text{-BINAP})(cod)]BF_4$ has been applied as a precatalyst in the asymmetric intramolecular [2+2+2] cycloaddition of enediynes, affording excellent enantiomeric excesses [Shibata *et al.* (2007). *J. Org. Chem.* **72**, 6521–6525].

3D view



Chemical scheme



Structure description

One of our main interests lies in the field of homogeneous asymmetric catalysis, with a special focus on asymmetric hydrogenation promoted by chiral rhodium bisphosphine complexes. A well known chiral ligand that forms seven-membered ring chelates is BINAP (Miyashita *et al.*, 1980).

A novel ligand, H_8-BINAP, developed recently by Takaya *et al.*, is able to coordinate to rhodium, affording a seven-membered chelate complex (Zhang *et al.*, 1994). The structure of the cod rhodium perchlorate complex $[Rh(H_8\text{-BINAP})(cod)]ClO_4$ containing the H_8-BINAP ligand is described in this article.

The title compound, $[Rh(H_8\text{-BINAP})(cod)]BF_4$, crystallizes in the Sohncke space group $P2_1$ as red prisms. This is isomorphous to the related perchlorate complex $[Rh(H_8\text{-BINAP})(cod)]ClO_4$ (Zhang *et al.*, 1994). The cationic complex of rhodium(I) is coordi-

Table 1
Selected distances (Å) and angles (°) of the rhodium/H_8-BINAP cod complexes (C_M = centroids of the double bonds of the olefin).

Complex	Rh—P	Rh—C_M	P—Rh—P	C_M—Rh—C_M
[[Rh(H_8-BINAP)(cod)]BF_4	2.3187 (6), 2.3343 (6)	2.116 (4), 2.140 (4)	91.055 (9)	83.80 (3)
[Rh(H_8-BINAP)(cod)]ClO_4	2.326, 2.337	2.143, 2.245	90.58	84.66

nated by a H_8-BINAP ligand and by a cycloocta-1,5-diene ligand in an η^2,η^2 fashion (Fig. 1). The asymmetric unit contains one cation, one anion, and cocrystallized pentane (0.72) and methanol (2 × 0.28) molecules.

The P—Rh—P bite angles is 91.055 (19)° for [Rh(H_8-BINAP)(cod)]BF_4 and 90.58° for [Rh(H_8-BINAP)(cod)]ClO_4 (Table 1), and are in the same range as those found in the parent BINAP diolefin complexes [Rh(BINAP)(diolefin)]X (with diolefin = nbd, cod; X = BF_4, ClO_4, OTf) 88.7 (1)–91.8 (1)° (Preetz *et al.*, 2011, and references therein). Comparable distances, *e.g.* Rh—P (Table 1), are also similar. The dihedral angles between the P/Rh/P and C_M/Rh/C_M planes (C_M = centroid of the double bond) are 1.98 (7)° for the title compound and 1.99° for the perchlorate rhodium complex. In general, this value is smaller for the rhodium H_8-BINAP complexes than for the related rhodium BINAP complexes 7.5–16.8° {an exception is the [Rh(BINAP)-(nbd)](OTf) complex with 0.3°} (Preetz *et al.*, 2010).

The application of [Rh(H_8-BINAP)(cod)]BF_4 as a precatalyst in the asymmetric intramolecular [2+2+2] cycloaddidion of enediynes leads to an excellent enantiomeric excesses (up to 98 ee%) (Shibata *et al.*, 2007). Hydrogenation of the cod is necessary to obtain the active catalyst.

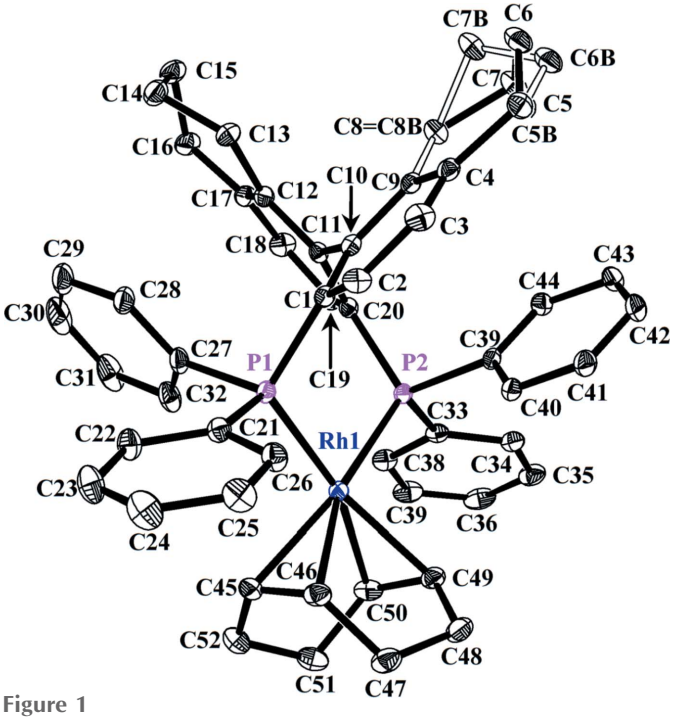


Figure 1
A view of the [Rh(H_8-BINAP)(cod)]$^+$ cation, with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity.

To determine the prehydrogenation time, catalytic hydrogenations of cod and nbd (norbornadiene) with [Rh(H_8-BINAP)(cod)]BF_4 or [Rh(H_8-BINAP)(nbd)]BF_4, respectively, have been carried out in MeOH according to Heller *et al.* (Drexler *et al.*, 2007).

Pseudo-rate constants were determined from the slope of the hydrogen consumption from the linear part of the curve – which represents the hydrogenation of the first double bond of the diolefin. Fig. 2 shows the hydrogen consumption curves for the catalytic hydrogenation of the first double bond with a high excess of cod and nbd. For the hydrogenation of nbd, we found 57.5 min^{-1} and for cod 0.851 min^{-1}. This gives a ratio of k'_{2nnbd}/k'_{2cod} of 67.6. The rate constants are slightly higher than those observed for BINAP rhodium complexes (27/0.23 min^{-1}) (Meissner *et al.*, 2014).

Synthesis and crystallization

All manipulations were carried out with standard Schlenk techniques under argon. NMR spectra were recorded on a Bruker ARX-300 spectrometer. Hydrogen consumptions were monitored using the device described in Drexler *et al.* (2007).

The cationic complexes [Rh(H_8-BINAP)(cod)]BF_4 and [Rh(H_8-BINAP)(nbd)]BF_4 were prepared by reaction of [Rh(diolefin)(acac)] and H_8-BINAP followed by addition of HBF_4 to the resulting solution, according to a modification of

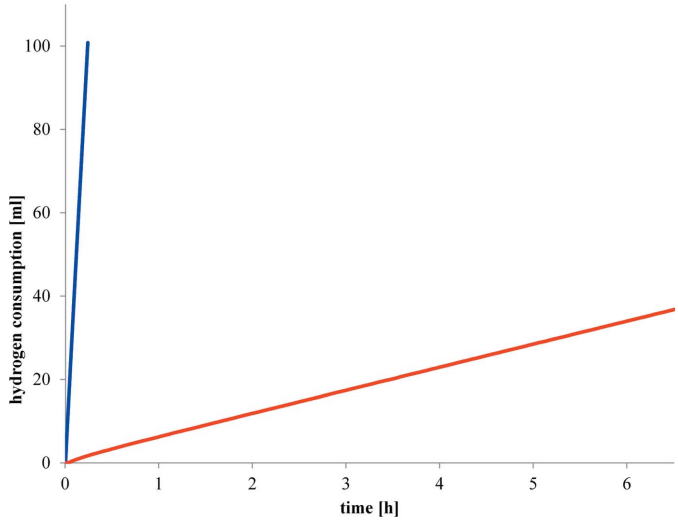


Figure 2
First part (first double bond) of the hydrogen consumption for the hydrogenation 0.0050 mmol [Rh(H_8-BINAP)(nbd)](BF_4), 4.77 mmol nb d, 15.0 ml MeOH, 298 K, normal pressure (blue) and 0.0044 mmol [Rh(H_8-BINAP)(cod)](BF_4), 1.84 mmol cod, 15.0 ml MeOH, 298 K, normal pressure (red).

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Rh(C_8H_{12})(C_{44}H_{20}P_2)]BF_4 \cdot 0.72C_5H_{12} \cdot 0.56CH_4O$
M_r	998.48
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	150
a, b, c (Å)	11.0916 (2), 15.3047 (3), 14.1459 (3)
β (°)	94.260 (1)
V (Å^3)	2394.68 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.48
Crystal size (mm)	0.50 × 0.42 × 0.22
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.686, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	125039, 10991, 10761
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.019, 0.049, 1.04
No. of reflections	10991
No. of parameters	685
No. of restraints	260
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.30
Absolute structure	Flack x determined using 5105 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.008 (3)

Computer programs: *APEX2* (Bruker, 2014), *SAINT* (Bruker, 2013), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

a previously published procedure (Schrock & Osborn, 1971). By overlaying a solution of $[Rh(H_8\text{-BINAP})(cod)]BF_4$ in methanol with pentane, red single crystals suitable for X-ray analysis were obtained.

^{31}P NMR (MeOH-d_4, 298 K, 121 MHz): $[Rh(H_8\text{-BINAP})(cod)]BF_4$: δ 24.7 (d, $J_{P\text{-}Rh}$ = 145.8 Hz); $[Rh(H_8\text{-BINAP})(nbd)]BF_4$: δ 25.4 (d, $J_{P\text{-}Rh}$ = 155.9 Hz).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The absolute configuration *R* for the title compound was determined using 5105 quotients in the refinement. The Flack parameter at convergence was −0.008 (3).

After refinement of the BF_4^- anion in $[Rh(H_8\text{-BINAP})(cod)]BF_4$, residual electron density and large anisotropic displacement parameters indicated an alternative orientation for this moiety. The occupancy of the alternative orientations was refined and their sum was constrained to unity; refinement converged for a ratio of 0.535 (8):0.465 (8) between the major and minor orientation. Restraints were used to equalize the bond lengths to improve the geometry and give similar U_{ij} components for the disordered BF_4^- anion.

Atoms C6 and C7 are disordered and were split, together with their neighbouring C5 and C8 atoms, in alternative positions, with an occupancy ratio of 0.727 (5):0273 (5), and were restrained to have similar U_{ij} components.

The solvent molecules share one position with a pentane–methanol ratio of 0.720 (4):[2 × 0.280 (4)] and were also restrained have similar U_{ij} components. The C—O distances in the methanol molecules were restrained to target values of 1.44 Å. The C—C distances in the pentane molecules were restrained to be similar.

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full crystallographic data

IUCrData (2017). **2**, x171240 [https://doi.org/10.1107/S2414314617012408]

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Crystal data

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M_r = 998.48
Monoclinic, $P2_1$
a = 11.0916 (2) Å
b = 15.3047 (3) Å
c = 14.1459 (3) Å
β = 94.260 (1)°
V = 2394.68 (8) Å^3
Z = 2
$F(000)$ = 1041
D_x = 1.385 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9769 reflections
θ = 2.3–27.5°
μ = 0.48 mm^{-1}
T = 150 K
Prism, red
0.50 × 0.42 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.686, T_{max} = 0.746
125039 measured reflections
10991 independent reflections
10761 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 27.5°, θ_{min} = 1.4°
h = −14→14
k = −19→19
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.049
S = 1.04
10991 reflections
685 parameters
260 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2 + 0.6009P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Absolute structure: Flack x determined using 5105 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.008 (3)

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Rh1	0.82304 (2)	0.75126 (2)	0.80792 (2)	0.01878 (4)	
P1	0.74750 (5)	0.82768 (4)	0.67490 (4)	0.01918 (10)	
P2	0.84440 (5)	0.88047 (3)	0.89523 (4)	0.01791 (10)	
C1	0.64594 (19)	0.91929 (14)	0.69716 (15)	0.0201 (4)	
C2	0.5207 (2)	0.90898 (16)	0.68133 (17)	0.0264 (5)	
H2	0.4892	0.8607	0.6452	0.032*	
C3	0.4425 (2)	0.96830 (17)	0.71766 (18)	0.0291 (5)	
H3	0.3579	0.9594	0.7069	0.035*	
C4	0.4843 (2)	1.04049 (16)	0.76942 (16)	0.0244 (4)	
C5	0.3906 (8)	1.0986 (9)	0.8093 (15)	0.0285 (16)	0.720 (4)
H5A	0.3654	1.0730	0.8690	0.034*	0.720 (4)
H5B	0.3185	1.1019	0.7638	0.034*	0.720 (4)
C6	0.4394 (3)	1.1894 (3)	0.8284 (3)	0.0334 (8)	0.720 (4)
H6A	0.3815	1.2236	0.8635	0.040*	0.720 (4)
H6B	0.4501	1.2196	0.7677	0.040*	0.720 (4)
C7	0.5611 (3)	1.1837 (2)	0.8869 (3)	0.0326 (7)	0.720 (4)
H7A	0.5893	1.2433	0.9044	0.039*	0.720 (4)
H7B	0.5506	1.1510	0.9461	0.039*	0.720 (4)
C8	0.6557 (2)	1.13826 (16)	0.83163 (17)	0.0271 (5)	0.720 (4)
H8A	0.6845	1.1795	0.7843	0.033*	0.720 (4)
H8B	0.7258	1.1226	0.8759	0.033*	0.720 (4)
C5B	0.402 (2)	1.102 (2)	0.820 (4)	0.0285 (16)	0.280 (4)
H5C	0.3407	1.1246	0.7713	0.034*	0.280 (4)
H5D	0.3581	1.0665	0.8644	0.034*	0.280 (4)
C6B	0.4524 (9)	1.1816 (7)	0.8755 (8)	0.0334 (8)	0.280 (4)
H6C	0.3902	1.2279	0.8756	0.040*	0.280 (4)
H6D	0.4754	1.1647	0.9419	0.040*	0.280 (4)
C7B	0.5621 (8)	1.2150 (6)	0.8290 (7)	0.0326 (7)	0.280 (4)
H7C	0.5970	1.2662	0.8639	0.039*	0.280 (4)
H7D	0.5394	1.2326	0.7627	0.039*	0.280 (4)
C8B	0.6557 (2)	1.13826 (16)	0.83163 (17)	0.0271 (5)	0.280 (4)
H8C	0.7291	1.1583	0.8022	0.033*	0.280 (4)
H8D	0.6796	1.1236	0.8986	0.033*	0.280 (4)
C9	0.60854 (19)	1.05614 (14)	0.78088 (15)	0.0207 (4)	
C10	0.68938 (19)	0.99491 (14)	0.74490 (15)	0.0196 (4)	
C11	0.82155 (18)	1.01648 (14)	0.75959 (15)	0.0191 (4)	
C12	0.86869 (19)	1.08103 (14)	0.70159 (15)	0.0217 (4)	
C13	0.7911 (2)	1.11869 (16)	0.61848 (16)	0.0263 (4)	
H13A	0.7300	1.1581	0.6432	0.032*	

H13B	0.7472	1.0703	0.5846	0.032*
C14	0.8620 (2)	1.16937 (18)	0.54775 (18)	0.0331 (5)
H14A	0.9050	1.1278	0.5085	0.040*
H14B	0.8053	1.2037	0.5051	0.040*
C15	0.9530 (2)	1.23048 (15)	0.5990 (2)	0.0332 (6)
H15A	0.9106	1.2715	0.6393	0.040*
H15B	0.9950	1.2650	0.5523	0.040*
C16	1.0447 (2)	1.17733 (17)	0.6602 (2)	0.0321 (5)
H16A	1.0979	1.1457	0.6186	0.039*
H16B	1.0959	1.2176	0.7006	0.039*
C17	0.9862 (2)	1.11201 (15)	0.72283 (17)	0.0253 (4)
C18	1.0511 (2)	1.08231 (17)	0.80484 (19)	0.0296 (5)
H18	1.1274	1.1078	0.8233	0.036*
C19	1.0069 (2)	1.01666 (16)	0.85966 (17)	0.0262 (4)
H19	1.0540	0.9963	0.9141	0.031*
C20	0.89329 (18)	0.97999 (14)	0.83567 (15)	0.0197 (4)
C21	0.66148 (18)	0.75831 (19)	0.58804 (14)	0.0239 (4)
C22	0.7066 (2)	0.73540 (17)	0.50185 (16)	0.0307 (6)
H22	0.7801	0.7604	0.4842	0.037*
C23	0.6440 (3)	0.6759 (2)	0.44154 (19)	0.0396 (6)
H23	0.6761	0.6598	0.3836	0.047*
C24	0.5358 (3)	0.6400 (2)	0.4653 (2)	0.0429 (7)
H24	0.4927	0.6007	0.4233	0.051*
C25	0.4909 (2)	0.66176 (19)	0.5506 (2)	0.0352 (6)
H25	0.4163	0.6377	0.5670	0.042*
C26	0.5540 (2)	0.71860 (17)	0.61255 (18)	0.0287 (5)
H26	0.5241	0.7308	0.6724	0.034*
C27	0.8710 (2)	0.87183 (15)	0.61120 (17)	0.0270 (5)
C28	0.9896 (2)	0.85627 (18)	0.64660 (19)	0.0346 (6)
H28	1.0053	0.8213	0.7016	0.041*
C29	1.0854 (3)	0.8923 (2)	0.6008 (3)	0.0503 (9)
H29	1.1663	0.8828	0.6257	0.060*
C30	1.0637 (4)	0.9411 (2)	0.5207 (3)	0.0601 (11)
H30	1.1293	0.9658	0.4904	0.072*
C31	0.9461 (4)	0.95470 (19)	0.4834 (2)	0.0523 (9)
H31	0.9316	0.9876	0.4268	0.063*
C32	0.8490 (3)	0.92039 (17)	0.52838 (19)	0.0369 (6)
H32	0.7684	0.9300	0.5028	0.044*
C33	0.9548 (2)	0.86850 (14)	0.99747 (16)	0.0221 (4)
C34	0.9212 (2)	0.86878 (15)	1.09020 (17)	0.0263 (4)
H34	0.8395	0.8800	1.1024	0.032*
C35	1.0070 (3)	0.85256 (17)	1.16552 (18)	0.0345 (6)
H35	0.9835	0.8529	1.2287	0.041*
C36	1.1260 (3)	0.83602 (18)	1.1485 (2)	0.0384 (6)
H36	1.1842	0.8255	1.1999	0.046*
C37	1.1599 (2)	0.83480 (18)	1.0566 (2)	0.0356 (6)
H37	1.2416	0.8232	1.0450	0.043*
C38	1.0753 (2)	0.85041 (16)	0.98093 (18)	0.0285 (5)

H38	1.0993	0.8488	0.9179	0.034*	
C39	0.7030 (2)	0.90642 (15)	0.94537 (16)	0.0206 (4)	
C40	0.6040 (2)	0.85126 (15)	0.92366 (15)	0.0226 (4)	
H40	0.6122	0.8022	0.8835	0.027*	
C41	0.4933 (2)	0.86829 (17)	0.96094 (18)	0.0289 (5)	
H41	0.4257	0.8315	0.9454	0.035*	
C42	0.4827 (2)	0.93896 (18)	1.02050 (19)	0.0333 (5)	
H42	0.4079	0.9497	1.0470	0.040*	
C43	0.5796 (2)	0.99438 (17)	1.04220 (18)	0.0317 (5)	
H43	0.5710	1.0429	1.0830	0.038*	
C44	0.6896 (2)	0.97870 (16)	1.00391 (16)	0.0256 (4)	
H44	0.7557	1.0173	1.0176	0.031*	
C45	0.8571 (3)	0.63513 (16)	0.71861 (17)	0.0312 (5)	
H45	0.854 (3)	0.658 (2)	0.6563 (13)	0.037*	
C46	0.7485 (2)	0.62307 (16)	0.75734 (17)	0.0289 (5)	
H46	0.6797 (19)	0.638 (2)	0.7163 (19)	0.035*	
C47	0.7242 (3)	0.56199 (17)	0.83809 (19)	0.0341 (5)	
H47A	0.7828	0.5131	0.8394	0.041*	
H47B	0.6421	0.5371	0.8266	0.041*	
C48	0.7341 (3)	0.60797 (18)	0.9345 (2)	0.0343 (6)	
H48A	0.6557	0.6359	0.9448	0.041*	
H48B	0.7503	0.5637	0.9849	0.041*	
C49	0.8322 (2)	0.67644 (16)	0.94369 (16)	0.0286 (5)	
H49	0.825 (3)	0.7198 (16)	0.9912 (17)	0.034*	
C50	0.9438 (2)	0.66987 (16)	0.90917 (18)	0.0298 (5)	
H50	1.002 (2)	0.7099 (17)	0.933 (2)	0.036*	
C51	0.9928 (3)	0.59022 (19)	0.8617 (2)	0.0389 (6)	
H51A	0.9510	0.5375	0.8834	0.047*	
H51B	1.0799	0.5842	0.8812	0.047*	
C52	0.9760 (3)	0.5953 (2)	0.7534 (2)	0.0419 (7)	
H52A	1.0424	0.6304	0.7298	0.050*	
H52B	0.9814	0.5357	0.7269	0.050*	
B1	0.3031 (12)	0.7140 (7)	0.7996 (7)	0.057 (3)	0.465 (8)
F1	0.4258 (13)	0.7105 (12)	0.8181 (14)	0.067 (4)	0.465 (8)
F2	0.2657 (7)	0.6820 (9)	0.7125 (6)	0.110 (3)	0.465 (8)
F3	0.2551 (10)	0.6727 (7)	0.8737 (9)	0.097 (3)	0.465 (8)
F4	0.2698 (7)	0.8003 (5)	0.8041 (7)	0.094 (3)	0.465 (8)
B1′	0.3170 (10)	0.6974 (6)	0.7955 (6)	0.050 (2)	0.535 (8)
F1′	0.4392 (10)	0.6892 (9)	0.8172 (10)	0.052 (2)	0.535 (8)
F2′	0.2769 (4)	0.6183 (4)	0.7588 (6)	0.087 (2)	0.535 (8)
F3′	0.2536 (10)	0.7148 (7)	0.8722 (8)	0.106 (3)	0.535 (8)
F4′	0.2971 (5)	0.7590 (7)	0.7271 (7)	0.118 (3)	0.535 (8)
O71	0.4066 (17)	0.9398 (14)	0.4145 (13)	0.126 (7)	0.280 (4)
H71	0.3902	0.9265	0.4697	0.189*	0.280 (4)
C71	0.3348 (19)	0.889 (2)	0.348 (2)	0.114 (10)	0.280 (4)
H71A	0.3770	0.8824	0.2904	0.171*	0.280 (4)
H71B	0.2574	0.9189	0.3334	0.171*	0.280 (4)
H71C	0.3203	0.8317	0.3756	0.171*	0.280 (4)

O61	0.7249 (11)	0.9616 (14)	0.2888 (11)	0.100 (4)	0.280 (4)
H61	0.7470	1.0119	0.2735	0.150*	0.280 (4)
C61	0.5993 (7)	0.9633 (4)	0.3056 (4)	0.1080 (19)	0.280 (4)
H61A	0.5701	1.0238	0.3028	0.162*	0.280 (4)
H61B	0.5883	0.9389	0.3684	0.162*	0.280 (4)
H61C	0.5534	0.9285	0.2572	0.162*	0.280 (4)
C73	0.6896 (10)	0.9051 (6)	0.2781 (6)	0.098 (3)	0.720 (4)
H73A	0.7356	0.9330	0.2298	0.148*	0.720 (4)
H73B	0.6515	0.8517	0.2520	0.148*	0.720 (4)
H73C	0.7443	0.8904	0.3334	0.148*	0.720 (4)
C74	0.5993 (7)	0.9633 (4)	0.3056 (4)	0.1080 (19)	0.720 (4)
H74A	0.6377	1.0158	0.3355	0.130*	0.720 (4)
H74B	0.5481	0.9822	0.2490	0.130*	0.720 (4)
C75	0.5288 (9)	0.9228 (8)	0.3685 (10)	0.154 (4)	0.720 (4)
H75A	0.5337	0.9579	0.4275	0.184*	0.720 (4)
H75B	0.5659	0.8653	0.3845	0.184*	0.720 (4)
C76	0.3983 (12)	0.9077 (13)	0.3401 (13)	0.170 (5)	0.720 (4)
H76A	0.3555	0.9633	0.3246	0.204*	0.720 (4)
H76B	0.3874	0.8676	0.2852	0.204*	0.720 (4)
C77	0.3581 (8)	0.8689 (7)	0.4240 (8)	0.110 (3)	0.720 (4)
H77A	0.2748	0.8483	0.4116	0.164*	0.720 (4)
H77B	0.3613	0.9124	0.4750	0.164*	0.720 (4)
H77C	0.4106	0.8195	0.4431	0.164*	0.720 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Rh1	0.01974 (7)	0.01788 (7)	0.01896 (7)	−0.00079 (7)	0.00298 (5)	−0.00042 (7)
P1	0.0202 (2)	0.0204 (2)	0.0174 (2)	−0.00308 (19)	0.00387 (19)	−0.00066 (19)
P2	0.0161 (2)	0.0194 (2)	0.0184 (2)	−0.00075 (19)	0.00228 (18)	−0.00018 (19)
C1	0.0196 (9)	0.0221 (10)	0.0186 (9)	0.0001 (8)	0.0020 (7)	0.0026 (8)
C2	0.0226 (10)	0.0240 (11)	0.0319 (12)	−0.0017 (8)	−0.0031 (9)	0.0006 (9)
C3	0.0144 (9)	0.0334 (12)	0.0386 (13)	−0.0011 (9)	−0.0033 (9)	0.0045 (10)
C4	0.0204 (10)	0.0286 (11)	0.0242 (10)	0.0033 (8)	0.0028 (8)	0.0080 (8)
C5	0.018 (2)	0.0358 (18)	0.031 (5)	0.0054 (16)	0.003 (3)	0.0032 (14)
C6	0.0302 (16)	0.0332 (16)	0.037 (2)	0.0115 (12)	0.0025 (18)	−0.0035 (18)
C7	0.0295 (15)	0.0326 (17)	0.0357 (18)	0.0058 (13)	0.0024 (14)	−0.0112 (13)
C8	0.0239 (10)	0.0273 (11)	0.0302 (11)	0.0020 (9)	0.0023 (9)	−0.0049 (9)
C5B	0.018 (2)	0.0358 (18)	0.031 (5)	0.0054 (16)	0.003 (3)	0.0032 (14)
C6B	0.0302 (16)	0.0332 (16)	0.037 (2)	0.0115 (12)	0.0025 (18)	−0.0035 (18)
C7B	0.0295 (15)	0.0326 (17)	0.0357 (18)	0.0058 (13)	0.0024 (14)	−0.0112 (13)
C8B	0.0239 (10)	0.0273 (11)	0.0302 (11)	0.0020 (9)	0.0023 (9)	−0.0049 (9)
C9	0.0200 (10)	0.0227 (10)	0.0196 (9)	0.0008 (8)	0.0020 (7)	0.0046 (8)
C10	0.0180 (9)	0.0225 (10)	0.0182 (9)	−0.0014 (8)	0.0012 (7)	0.0036 (7)
C11	0.0164 (9)	0.0193 (9)	0.0221 (10)	−0.0019 (7)	0.0042 (7)	−0.0025 (8)
C12	0.0209 (10)	0.0212 (10)	0.0234 (10)	−0.0003 (8)	0.0044 (8)	0.0008 (8)
C13	0.0261 (11)	0.0258 (11)	0.0269 (11)	−0.0031 (9)	0.0014 (8)	0.0052 (9)
C14	0.0393 (13)	0.0318 (13)	0.0287 (12)	−0.0035 (11)	0.0055 (10)	0.0048 (10)

C15	0.0349 (12)	0.0269 (14)	0.0384 (13)	−0.0056 (9)	0.0066 (10)	0.0087 (9)
C16	0.0258 (11)	0.0279 (12)	0.0438 (14)	−0.0053 (9)	0.0096 (10)	0.0087 (10)
C17	0.0199 (10)	0.0222 (10)	0.0346 (12)	−0.0016 (8)	0.0078 (8)	0.0039 (9)
C18	0.0179 (10)	0.0297 (12)	0.0409 (13)	−0.0056 (9)	0.0001 (9)	0.0032 (10)
C19	0.0199 (10)	0.0272 (11)	0.0310 (11)	−0.0015 (8)	−0.0018 (8)	0.0021 (9)
C20	0.0174 (9)	0.0196 (10)	0.0226 (10)	−0.0015 (7)	0.0042 (7)	−0.0006 (8)
C21	0.0259 (9)	0.0249 (11)	0.0205 (8)	−0.0011 (11)	−0.0009 (7)	−0.0010 (10)
C22	0.0311 (11)	0.0378 (17)	0.0233 (10)	−0.0029 (10)	0.0019 (8)	−0.0058 (9)
C23	0.0396 (14)	0.0521 (17)	0.0265 (12)	−0.0009 (13)	−0.0008 (10)	−0.0148 (12)
C24	0.0384 (14)	0.0485 (17)	0.0400 (15)	−0.0066 (13)	−0.0091 (11)	−0.0178 (13)
C25	0.0267 (12)	0.0375 (14)	0.0406 (14)	−0.0063 (10)	−0.0038 (10)	−0.0061 (11)
C26	0.0285 (12)	0.0293 (11)	0.0285 (11)	−0.0054 (9)	0.0043 (9)	−0.0056 (9)
C27	0.0310 (11)	0.0259 (11)	0.0259 (11)	−0.0082 (9)	0.0134 (9)	−0.0062 (9)
C28	0.0295 (12)	0.0378 (14)	0.0381 (13)	−0.0101 (10)	0.0141 (10)	−0.0135 (11)
C29	0.0358 (15)	0.0528 (18)	0.066 (2)	−0.0217 (14)	0.0280 (14)	−0.0252 (16)
C30	0.069 (2)	0.0457 (18)	0.073 (2)	−0.0285 (17)	0.053 (2)	−0.0211 (17)
C31	0.090 (3)	0.0296 (14)	0.0422 (16)	−0.0148 (15)	0.0405 (17)	−0.0056 (12)
C32	0.0573 (17)	0.0269 (12)	0.0291 (12)	−0.0066 (11)	0.0202 (12)	−0.0013 (10)
C33	0.0231 (10)	0.0182 (10)	0.0242 (10)	−0.0018 (8)	−0.0037 (8)	0.0000 (8)
C34	0.0301 (11)	0.0222 (11)	0.0261 (11)	−0.0003 (9)	−0.0012 (9)	0.0020 (8)
C35	0.0480 (15)	0.0289 (12)	0.0250 (12)	0.0011 (11)	−0.0076 (10)	0.0044 (10)
C36	0.0403 (14)	0.0304 (13)	0.0412 (15)	−0.0016 (11)	−0.0182 (11)	0.0087 (11)
C37	0.0244 (11)	0.0301 (13)	0.0506 (16)	0.0005 (10)	−0.0079 (10)	0.0063 (11)
C38	0.0241 (11)	0.0257 (11)	0.0352 (12)	−0.0011 (9)	−0.0005 (9)	0.0023 (9)
C39	0.0198 (10)	0.0245 (11)	0.0178 (10)	0.0016 (8)	0.0038 (8)	0.0042 (8)
C40	0.0220 (10)	0.0238 (10)	0.0226 (10)	0.0004 (8)	0.0059 (8)	0.0026 (8)
C41	0.0230 (11)	0.0325 (12)	0.0322 (12)	0.0003 (9)	0.0083 (9)	0.0044 (10)
C42	0.0282 (12)	0.0390 (13)	0.0345 (13)	0.0092 (10)	0.0146 (10)	0.0035 (11)
C43	0.0372 (13)	0.0319 (12)	0.0269 (12)	0.0097 (10)	0.0092 (10)	−0.0014 (9)
C44	0.0277 (11)	0.0266 (11)	0.0228 (10)	0.0027 (9)	0.0030 (8)	0.0003 (9)
C45	0.0477 (15)	0.0218 (11)	0.0244 (11)	0.0043 (10)	0.0057 (10)	−0.0028 (9)
C46	0.0373 (13)	0.0212 (11)	0.0273 (11)	−0.0043 (9)	−0.0034 (9)	−0.0027 (9)
C47	0.0416 (14)	0.0250 (12)	0.0354 (13)	−0.0091 (10)	−0.0002 (11)	0.0028 (10)
C48	0.0447 (16)	0.0283 (13)	0.0301 (13)	−0.0053 (11)	0.0044 (11)	0.0066 (10)
C49	0.0414 (13)	0.0225 (11)	0.0216 (11)	−0.0009 (10)	0.0006 (9)	0.0014 (9)
C50	0.0325 (12)	0.0217 (11)	0.0338 (12)	0.0002 (9)	−0.0075 (10)	0.0005 (9)
C51	0.0366 (14)	0.0298 (13)	0.0496 (16)	0.0107 (11)	−0.0016 (12)	0.0003 (11)
C52	0.0438 (15)	0.0362 (14)	0.0473 (16)	0.0141 (12)	0.0145 (13)	−0.0012 (12)
B1	0.038 (5)	0.061 (5)	0.075 (6)	−0.012 (4)	0.011 (5)	−0.015 (5)
F1	0.045 (5)	0.083 (9)	0.076 (5)	−0.007 (4)	0.020 (4)	−0.033 (5)
F2	0.087 (4)	0.156 (9)	0.084 (5)	0.009 (5)	−0.016 (4)	−0.050 (5)
F3	0.068 (4)	0.111 (7)	0.117 (6)	−0.009 (5)	0.032 (4)	0.050 (6)
F4	0.081 (5)	0.089 (5)	0.111 (6)	0.004 (4)	−0.001 (4)	0.009 (4)
B1′	0.040 (4)	0.049 (4)	0.062 (4)	0.003 (3)	0.013 (4)	−0.003 (3)
F1′	0.036 (3)	0.069 (6)	0.052 (4)	−0.002 (3)	0.013 (2)	0.005 (4)
F2′	0.050 (3)	0.078 (4)	0.133 (5)	−0.009 (2)	0.006 (3)	−0.040 (4)
F3′	0.078 (4)	0.132 (7)	0.117 (5)	−0.013 (5)	0.062 (4)	−0.054 (5)
F4′	0.076 (3)	0.119 (6)	0.157 (7)	0.014 (4)	−0.004 (4)	0.058 (6)

O71	0.138 (16)	0.152 (18)	0.090 (11)	−0.023 (13)	0.016 (10)	−0.034 (11)
C71	0.056 (11)	0.16 (3)	0.115 (18)	0.014 (14)	−0.047 (12)	0.002 (19)
O61	0.104 (9)	0.124 (11)	0.070 (7)	0.011 (9)	−0.006 (7)	0.008 (9)
C61	0.155 (5)	0.088 (4)	0.087 (4)	0.022 (4)	0.046 (4)	0.019 (3)
C73	0.160 (8)	0.077 (5)	0.058 (4)	0.017 (5)	0.008 (5)	0.000 (4)
C74	0.155 (5)	0.088 (4)	0.087 (4)	0.022 (4)	0.046 (4)	0.019 (3)
C75	0.129 (7)	0.125 (7)	0.207 (9)	0.004 (6)	0.013 (7)	0.035 (7)
C76	0.152 (10)	0.155 (10)	0.194 (11)	−0.025 (9)	−0.048 (10)	0.055 (9)
C77	0.080 (5)	0.096 (6)	0.150 (9)	0.003 (5)	−0.011 (6)	0.019 (6)

Geometric parameters (Å, º)

Rh1—C46	2.226 (2)	C29—C30	1.364 (6)
Rh1—C45	2.229 (2)	C29—H29	0.9500
Rh1—C49	2.232 (2)	C30—C31	1.386 (6)
Rh1—C50	2.261 (2)	C30—H30	0.9500
Rh1—P1	2.3187 (6)	C31—C32	1.394 (4)
Rh1—P2	2.3343 (6)	C31—H31	0.9500
P1—C27	1.824 (2)	C32—H32	0.9500
P1—C21	1.837 (2)	C33—C34	1.390 (3)
P1—C1	1.840 (2)	C33—C38	1.402 (3)
P2—C39	1.812 (2)	C34—C35	1.398 (3)
P2—C33	1.833 (2)	C34—H34	0.9500
P2—C20	1.842 (2)	C35—C36	1.382 (4)
C1—C2	1.399 (3)	C35—H35	0.9500
C1—C10	1.407 (3)	C36—C37	1.379 (4)
C2—C3	1.381 (3)	C36—H36	0.9500
C2—H2	0.9500	C37—C38	1.391 (4)
C3—C4	1.386 (4)	C37—H37	0.9500
C3—H3	0.9500	C38—H38	0.9500
C4—C9	1.397 (3)	C39—C44	1.396 (3)
C4—C5	1.509 (8)	C39—C40	1.401 (3)
C4—C5B	1.53 (2)	C40—C41	1.396 (3)
C5—C6	1.509 (11)	C40—H40	0.9500
C5—H5A	0.9900	C41—C42	1.381 (4)
C5—H5B	0.9900	C41—H41	0.9500
C6—C7	1.532 (5)	C42—C43	1.386 (4)
C6—H6A	0.9900	C42—H42	0.9500
C6—H6B	0.9900	C43—C44	1.392 (3)
C7—C8	1.523 (4)	C43—H43	0.9500
C7—H7A	0.9900	C44—H44	0.9500
C7—H7B	0.9900	C45—C46	1.372 (4)
C8—C9	1.521 (3)	C45—C52	1.503 (4)
C8—H8A	0.9900	C45—H45	0.946 (14)
C8—H8B	0.9900	C46—C47	1.516 (3)
C5B—C6B	1.53 (2)	C46—H46	0.953 (13)
C5B—H5C	0.9900	C47—C48	1.532 (4)
C5B—H5D	0.9900	C47—H47A	0.9900

C6B—C7B	1.514 (13)	C47—H47B	0.9900
C6B—H6C	0.9900	C48—C49	1.509 (4)
C6B—H6D	0.9900	C48—H48A	0.9900
C7B—H7C	0.9900	C48—H48B	0.9900
C7B—H7D	0.9900	C49—C50	1.368 (4)
C9—C10	1.417 (3)	C49—H49	0.952 (14)
C10—C11	1.502 (3)	C50—C51	1.512 (4)
C11—C20	1.406 (3)	C50—H50	0.939 (14)
C11—C12	1.409 (3)	C51—C52	1.531 (4)
C12—C17	1.398 (3)	C51—H51A	0.9900
C12—C13	1.518 (3)	C51—H51B	0.9900
C13—C14	1.529 (3)	C52—H52A	0.9900
C13—H13A	0.9900	C52—H52B	0.9900
C13—H13B	0.9900	B1—F2	1.362 (9)
C14—C15	1.520 (4)	B1—F3	1.366 (9)
C14—H14A	0.9900	B1—F1	1.368 (9)
C14—H14B	0.9900	B1—F4	1.375 (9)
C15—C16	1.522 (4)	B1′—F4′	1.357 (8)
C15—H15A	0.9900	B1′—F3′	1.362 (8)
C15—H15B	0.9900	B1′—F1′	1.374 (8)
C16—C17	1.514 (3)	B1′—F2′	1.377 (9)
C16—H16A	0.9900	O71—C71	1.411 (13)
C16—H16B	0.9900	O71—H71	0.8400
C17—C18	1.395 (4)	C71—H71A	0.9800
C18—C19	1.381 (3)	C71—H71B	0.9800
C18—H18	0.9500	C71—H71C	0.9800
C19—C20	1.398 (3)	O61—C61	1.431 (11)
C19—H19	0.9500	O61—H61	0.8400
C21—C22	1.397 (3)	C61—H61A	0.9800
C21—C26	1.405 (3)	C61—H61B	0.9800
C22—C23	1.397 (4)	C61—H61C	0.9800
C22—H22	0.9500	C73—H73A	0.9800
C23—C24	1.384 (4)	C73—H73B	0.9800
C23—H23	0.9500	C73—H73C	0.9800
C24—C25	1.380 (4)	C75—C76	1.491 (15)
C24—H24	0.9500	C75—H75A	0.9900
C25—C26	1.387 (4)	C75—H75B	0.9900
C25—H25	0.9500	C76—C77	1.428 (15)
C26—H26	0.9500	C76—H76A	0.9900
C27—C28	1.392 (4)	C76—H76B	0.9900
C27—C32	1.394 (4)	C77—H77A	0.9800
C28—C29	1.399 (4)	C77—H77B	0.9800
C28—H28	0.9500	C77—H77C	0.9800

C46—Rh1—C45	35.86 (10)	C28—C27—C32	119.7 (2)
C46—Rh1—C49	79.42 (9)	C28—C27—P1	118.86 (19)
C45—Rh1—C49	94.58 (9)	C32—C27—P1	121.4 (2)
C46—Rh1—C50	84.63 (9)	C27—C28—C29	119.7 (3)

C45—Rh1—C50	78.61 (9)	C27—C28—H28	120.1
C49—Rh1—C50	35.44 (10)	C29—C28—H28	120.1
C46—Rh1—P1	94.63 (7)	C30—C29—C28	120.5 (3)
C45—Rh1—P1	90.48 (7)	C30—C29—H29	119.8
C49—Rh1—P1	161.39 (7)	C28—C29—H29	119.8
C50—Rh1—P1	162.43 (7)	C29—C30—C31	120.1 (3)
C46—Rh1—P2	159.61 (7)	C29—C30—H30	119.9
C45—Rh1—P2	163.86 (7)	C31—C30—H30	119.9
C49—Rh1—P2	89.02 (6)	C30—C31—C32	120.5 (3)
C50—Rh1—P2	95.71 (7)	C30—C31—H31	119.8
P1—Rh1—P2	91.055 (19)	C32—C31—H31	119.8
C27—P1—C21	104.80 (10)	C27—C32—C31	119.4 (3)
C27—P1—C1	107.09 (10)	C27—C32—H32	120.3
C21—P1—C1	105.11 (11)	C31—C32—H32	120.3
C27—P1—Rh1	110.39 (9)	C34—C33—C38	118.9 (2)
C21—P1—Rh1	112.94 (9)	C34—C33—P2	122.28 (18)
C1—P1—Rh1	115.74 (7)	C38—C33—P2	118.50 (17)
C39—P2—C33	105.05 (10)	C33—C34—C35	120.2 (2)
C39—P2—C20	106.89 (10)	C33—C34—H34	119.9
C33—P2—C20	103.98 (10)	C35—C34—H34	119.9
C39—P2—Rh1	109.63 (8)	C36—C35—C34	120.3 (2)
C33—P2—Rh1	111.61 (7)	C36—C35—H35	119.8
C20—P2—Rh1	118.71 (7)	C34—C35—H35	119.8
C2—C1—C10	118.0 (2)	C37—C36—C35	119.8 (2)
C2—C1—P1	119.98 (17)	C37—C36—H36	120.1
C10—C1—P1	121.11 (16)	C35—C36—H36	120.1
C3—C2—C1	120.6 (2)	C36—C37—C38	120.5 (2)
C3—C2—H2	119.7	C36—C37—H37	119.7
C1—C2—H2	119.7	C38—C37—H37	119.7
C2—C3—C4	121.8 (2)	C37—C38—C33	120.2 (2)
C2—C3—H3	119.1	C37—C38—H38	119.9
C4—C3—H3	119.1	C33—C38—H38	119.9
C3—C4—C9	119.1 (2)	C44—C39—C40	119.4 (2)
C3—C4—C5	117.1 (4)	C44—C39—P2	122.61 (18)
C9—C4—C5	123.8 (4)	C40—C39—P2	117.98 (18)
C3—C4—C5B	123.6 (9)	C41—C40—C39	120.1 (2)
C9—C4—C5B	117.3 (10)	C41—C40—H40	119.9
C4—C5—C6	111.3 (7)	C39—C40—H40	119.9
C4—C5—H5A	109.4	C42—C41—C40	119.6 (2)
C6—C5—H5A	109.4	C42—C41—H41	120.2
C4—C5—H5B	109.4	C40—C41—H41	120.2
C6—C5—H5B	109.4	C41—C42—C43	121.0 (2)
H5A—C5—H5B	108.0	C41—C42—H42	119.5
C5—C6—C7	109.5 (7)	C43—C42—H42	119.5
C5—C6—H6A	109.8	C42—C43—C44	119.7 (2)
C7—C6—H6A	109.8	C42—C43—H43	120.1
C5—C6—H6B	109.8	C44—C43—H43	120.1
C7—C6—H6B	109.8	C43—C44—C39	120.2 (2)

H6A—C6—H6B	108.2	C43—C44—H44	119.9
C8—C7—C6	111.2 (3)	C39—C44—H44	119.9
C8—C7—H7A	109.4	C46—C45—C52	126.1 (2)
C6—C7—H7A	109.4	C46—C45—Rh1	71.96 (14)
C8—C7—H7B	109.4	C52—C45—Rh1	108.63 (18)
C6—C7—H7B	109.4	C46—C45—H45	117 (2)
H7A—C7—H7B	108.0	C52—C45—H45	115 (2)
C9—C8—C7	113.2 (2)	Rh1—C45—H45	104 (2)
C9—C8—H8A	108.9	C45—C46—C47	126.5 (2)
C7—C8—H8A	108.9	C45—C46—Rh1	72.18 (14)
C9—C8—H8B	108.9	C47—C46—Rh1	112.58 (16)
C7—C8—H8B	108.9	C45—C46—H46	114.2 (19)
H8A—C8—H8B	107.8	C47—C46—H46	116 (2)
C6B—C5B—C4	121.5 (17)	Rh1—C46—H46	104 (2)
C6B—C5B—H5C	106.9	C46—C47—C48	112.5 (2)
C4—C5B—H5C	106.9	C46—C47—H47A	109.1
C6B—C5B—H5D	106.9	C48—C47—H47A	109.1
C4—C5B—H5D	106.9	C46—C47—H47B	109.1
H5C—C5B—H5D	106.7	C48—C47—H47B	109.1
C7B—C6B—C5B	108.7 (17)	H47A—C47—H47B	107.8
C7B—C6B—H6C	110.0	C49—C48—C47	113.5 (2)
C5B—C6B—H6C	110.0	C49—C48—H48A	108.9
C7B—C6B—H6D	110.0	C47—C48—H48A	108.9
C5B—C6B—H6D	110.0	C49—C48—H48B	108.9
H6C—C6B—H6D	108.3	C47—C48—H48B	108.9
C6B—C7B—H7C	110.4	H48A—C48—H48B	107.7
C6B—C7B—H7D	110.4	C50—C49—C48	125.7 (2)
H7C—C7B—H7D	108.6	C50—C49—Rh1	73.44 (14)
C4—C9—C10	119.4 (2)	C48—C49—Rh1	107.23 (16)
C4—C9—C8	119.9 (2)	C50—C49—H49	115.4 (19)
C10—C9—C8	120.74 (19)	C48—C49—H49	116.6 (19)
C1—C10—C9	120.87 (19)	Rh1—C49—H49	104.5 (19)
C1—C10—C11	122.90 (19)	C49—C50—C51	125.6 (2)
C9—C10—C11	116.23 (19)	C49—C50—Rh1	71.11 (14)
C20—C11—C12	120.72 (19)	C51—C50—Rh1	112.22 (17)
C20—C11—C10	120.65 (18)	C49—C50—H50	116 (2)
C12—C11—C10	118.29 (19)	C51—C50—H50	115 (2)
C17—C12—C11	119.5 (2)	Rh1—C50—H50	103 (2)
C17—C12—C13	120.2 (2)	C50—C51—C52	112.5 (2)
C11—C12—C13	120.22 (19)	C50—C51—H51A	109.1
C12—C13—C14	114.2 (2)	C52—C51—H51A	109.1
C12—C13—H13A	108.7	C50—C51—H51B	109.1
C14—C13—H13A	108.7	C52—C51—H51B	109.1
C12—C13—H13B	108.7	H51A—C51—H51B	107.8
C14—C13—H13B	108.7	C45—C52—C51	112.7 (2)
H13A—C13—H13B	107.6	C45—C52—H52A	109.0
C15—C14—C13	110.8 (2)	C51—C52—H52A	109.0
C15—C14—H14A	109.5	C45—C52—H52B	109.0

C13—C14—H14A	109.5	C51—C52—H52B	109.0
C15—C14—H14B	109.5	H52A—C52—H52B	107.8
C13—C14—H14B	109.5	F2—B1—F3	114.7 (11)
H14A—C14—H14B	108.1	F2—B1—F1	113.0 (13)
C14—C15—C16	109.6 (2)	F3—B1—F1	105.9 (12)
C14—C15—H15A	109.8	F2—B1—F4	108.8 (10)
C16—C15—H15A	109.8	F3—B1—F4	106.7 (9)
C14—C15—H15B	109.8	F1—B1—F4	107.2 (10)
C16—C15—H15B	109.8	F4′—B1′—F3′	111.5 (10)
H15A—C15—H15B	108.2	F4′—B1′—F1′	109.2 (9)
C17—C16—C15	112.8 (2)	F3′—B1′—F1′	113.5 (10)
C17—C16—H16A	109.0	F4′—B1′—F2′	108.1 (9)
C15—C16—H16A	109.0	F3′—B1′—F2′	107.5 (8)
C17—C16—H16B	109.0	F1′—B1′—F2′	106.9 (9)
C15—C16—H16B	109.0	C71—O71—H71	109.5
H16A—C16—H16B	107.8	O71—C71—H71A	109.5
C18—C17—C12	118.9 (2)	O71—C71—H71B	109.5
C18—C17—C16	118.9 (2)	H71A—C71—H71B	109.5
C12—C17—C16	122.1 (2)	O71—C71—H71C	109.5
C19—C18—C17	121.4 (2)	H71A—C71—H71C	109.5
C19—C18—H18	119.3	H71B—C71—H71C	109.5
C17—C18—H18	119.3	C61—O61—H61	109.5
C18—C19—C20	120.5 (2)	O61—C61—H61A	109.4
C18—C19—H19	119.8	O61—C61—H61B	109.4
C20—C19—H19	119.8	H61A—C61—H61B	109.5
C19—C20—C11	118.4 (2)	O61—C61—H61C	109.6
C19—C20—P2	120.77 (17)	H61A—C61—H61C	109.5
C11—C20—P2	120.64 (16)	H61B—C61—H61C	109.5
C22—C21—C26	118.2 (2)	H73A—C73—H73B	109.5
C22—C21—P1	121.81 (17)	H73A—C73—H73C	109.5
C26—C21—P1	119.56 (16)	H73B—C73—H73C	109.5
C21—C22—C23	120.2 (2)	C76—C75—H75A	107.6
C21—C22—H22	119.9	C76—C75—H75B	107.6
C23—C22—H22	119.9	H75A—C75—H75B	107.0
C24—C23—C22	120.7 (3)	C77—C76—C75	101.4 (12)
C24—C23—H23	119.7	C77—C76—H76A	111.5
C22—C23—H23	119.7	C75—C76—H76A	111.5
C25—C24—C23	119.5 (3)	C77—C76—H76B	111.5
C25—C24—H24	120.2	C75—C76—H76B	111.5
C23—C24—H24	120.2	H76A—C76—H76B	109.3
C24—C25—C26	120.4 (3)	C76—C77—H77A	109.5
C24—C25—H25	119.8	C76—C77—H77B	109.5
C26—C25—H25	119.8	H77A—C77—H77B	109.5
C25—C26—C21	120.9 (2)	C76—C77—H77C	109.5
C25—C26—H26	119.6	H77A—C77—H77C	109.5
C21—C26—H26	119.6	H77B—C77—H77C	109.5
C27—P1—C1—C2	135.31 (19)	C27—P1—C21—C22	12.0 (3)

C21—P1—C1—C2	24.2 (2)	C1—P1—C21—C22	124.7 (2)
Rh1—P1—C1—C2	−101.12 (18)	Rh1—P1—C21—C22	−108.2 (2)
C27—P1—C1—C10	−55.60 (19)	C27—P1—C21—C26	−175.6 (2)
C21—P1—C1—C10	−166.69 (17)	C1—P1—C21—C26	−62.9 (2)
Rh1—P1—C1—C10	67.97 (18)	Rh1—P1—C21—C26	64.2 (2)
C10—C1—C2—C3	−4.6 (3)	C26—C21—C22—C23	1.3 (4)
P1—C1—C2—C3	164.83 (19)	P1—C21—C22—C23	173.9 (2)
C1—C2—C3—C4	1.1 (4)	C21—C22—C23—C24	1.1 (5)
C2—C3—C4—C9	3.4 (4)	C22—C23—C24—C25	−1.6 (5)
C2—C3—C4—C5	−177.3 (10)	C23—C24—C25—C26	−0.5 (5)
C2—C3—C4—C5B	−173 (3)	C24—C25—C26—C21	3.0 (4)
C3—C4—C5—C6	−157.3 (8)	C22—C21—C26—C25	−3.4 (4)
C9—C4—C5—C6	21.9 (19)	P1—C21—C26—C25	−176.1 (2)
C5B—C4—C5—C6	50 (22)	C21—P1—C27—C28	−122.0 (2)
C4—C5—C6—C7	−50.7 (15)	C1—P1—C27—C28	126.73 (19)
C5—C6—C7—C8	64.2 (8)	Rh1—P1—C27—C28	−0.1 (2)
C6—C7—C8—C9	−44.7 (4)	C21—P1—C27—C32	58.0 (2)
C3—C4—C5B—C6B	−180 (3)	C1—P1—C27—C32	−53.3 (2)
C9—C4—C5B—C6B	4 (6)	Rh1—P1—C27—C32	179.87 (18)
C5—C4—C5B—C6B	−150 (28)	C32—C27—C28—C29	2.5 (4)
C4—C5B—C6B—C7B	32 (5)	P1—C27—C28—C29	−177.6 (2)
C3—C4—C9—C10	−4.2 (3)	C27—C28—C29—C30	−1.3 (4)
C5—C4—C9—C10	176.6 (11)	C28—C29—C30—C31	−0.6 (5)
C5B—C4—C9—C10	173 (3)	C29—C30—C31—C32	1.4 (5)
C3—C4—C9—C8	175.8 (2)	C28—C27—C32—C31	−1.7 (4)
C5—C4—C9—C8	−3.3 (11)	P1—C27—C32—C31	178.4 (2)
C5B—C4—C9—C8	−7 (3)	C30—C31—C32—C27	−0.3 (4)
C7—C8—C9—C4	14.8 (3)	C39—P2—C33—C34	7.8 (2)
C7—C8—C9—C10	−165.2 (2)	C20—P2—C33—C34	119.89 (19)
C2—C1—C10—C9	3.7 (3)	Rh1—P2—C33—C34	−110.98 (18)
P1—C1—C10—C9	−165.56 (16)	C39—P2—C33—C38	−178.27 (18)
C2—C1—C10—C11	−175.3 (2)	C20—P2—C33—C38	−66.1 (2)
P1—C1—C10—C11	15.4 (3)	Rh1—P2—C33—C38	63.00 (19)
C4—C9—C10—C1	0.6 (3)	C38—C33—C34—C35	1.0 (3)
C8—C9—C10—C1	−179.4 (2)	P2—C33—C34—C35	174.93 (19)
C4—C9—C10—C11	179.74 (19)	C33—C34—C35—C36	−0.1 (4)
C8—C9—C10—C11	−0.3 (3)	C34—C35—C36—C37	−0.5 (4)
C1—C10—C11—C20	−83.5 (3)	C35—C36—C37—C38	0.2 (4)
C9—C10—C11—C20	97.4 (2)	C36—C37—C38—C33	0.7 (4)
C1—C10—C11—C12	103.2 (2)	C34—C33—C38—C37	−1.3 (4)
C9—C10—C11—C12	−75.9 (2)	P2—C33—C38—C37	−175.47 (19)
C20—C11—C12—C17	−3.1 (3)	C33—P2—C39—C44	57.7 (2)
C10—C11—C12—C17	170.3 (2)	C20—P2—C39—C44	−52.3 (2)
C20—C11—C12—C13	178.8 (2)	Rh1—P2—C39—C44	177.79 (17)
C10—C11—C12—C13	−7.8 (3)	C33—P2—C39—C40	−122.44 (18)
C17—C12—C13—C14	16.9 (3)	C20—P2—C39—C40	127.50 (18)
C11—C12—C13—C14	−165.0 (2)	Rh1—P2—C39—C40	−2.4 (2)
C12—C13—C14—C15	−45.3 (3)	C44—C39—C40—C41	−0.5 (3)

C13—C14—C15—C16	62.5 (3)	P2—C39—C40—C41	179.70 (18)
C14—C15—C16—C17	−50.2 (3)	C39—C40—C41—C42	−1.0 (4)
C11—C12—C17—C18	−4.2 (3)	C40—C41—C42—C43	1.4 (4)
C13—C12—C17—C18	173.9 (2)	C41—C42—C43—C44	−0.3 (4)
C11—C12—C17—C16	176.4 (2)	C42—C43—C44—C39	−1.3 (4)
C13—C12—C17—C16	−5.6 (3)	C40—C39—C44—C43	1.6 (3)
C15—C16—C17—C18	−156.8 (2)	P2—C39—C44—C43	−178.55 (19)
C15—C16—C17—C12	22.6 (3)	C52—C45—C46—C47	−5.0 (4)
C12—C17—C18—C19	6.8 (4)	Rh1—C45—C46—C47	−105.3 (2)
C16—C17—C18—C19	−173.7 (2)	C52—C45—C46—Rh1	100.3 (3)
C17—C18—C19—C20	−2.0 (4)	C45—C46—C47—C48	94.6 (3)
C18—C19—C20—C11	−5.3 (3)	Rh1—C46—C47—C48	10.6 (3)
C18—C19—C20—P2	169.38 (19)	C46—C47—C48—C49	−36.2 (3)
C12—C11—C20—C19	7.8 (3)	C47—C48—C49—C50	−39.1 (4)
C10—C11—C20—C19	−165.4 (2)	C47—C48—C49—Rh1	42.6 (3)
C12—C11—C20—P2	−166.86 (16)	C48—C49—C50—C51	−4.7 (4)
C10—C11—C20—P2	19.9 (3)	Rh1—C49—C50—C51	−104.3 (3)
C39—P2—C20—C19	123.92 (19)	C48—C49—C50—Rh1	99.6 (2)
C33—P2—C20—C19	13.1 (2)	C49—C50—C51—C52	96.5 (3)
Rh1—P2—C20—C19	−111.57 (17)	Rh1—C50—C51—C52	14.4 (3)
C39—P2—C20—C11	−61.52 (19)	C46—C45—C52—C51	−37.7 (4)
C33—P2—C20—C11	−172.33 (17)	Rh1—C45—C52—C51	43.2 (3)
Rh1—P2—C20—C11	62.99 (18)	C50—C51—C52—C45	−38.7 (4)