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trans-Carbonylchloridobis(ethyldiphenylphosphine-κP)rhodium(I)

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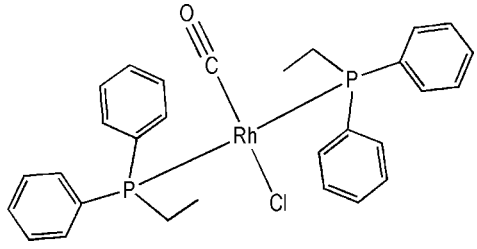
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.037; wR factor = 0.080; data-to-parameter ratio = 19.0.

The title compound, $[RhCl(C_{14}H_{15}P)_2(CO)]$, crystallizes with two almost identical molecules in the asymmetric unit. The molecules have the Rh^I atom in a square-planar geometry. The crystal structure involves intermolecular C—H···O hydrogen bonds.

Related literature

For related literature, see: Beck *et al.* (1999); Higham *et al.* (2004); Hoye *et al.* (1993); Lorenzini *et al.* (2007*a*,*b*,*c*); O'Connor & Wilkinson (1969); Vallarino (1957); Vaska & Di Luzio (1961, 1962).



Experimental

Crystal data

$[RhCl(C_{14}H_{15}P)_2(CO)]$
M_r = 594.83
Monoclinic, $P2_1$
a = 9.8557 (14) Å
b = 16.385 (2) Å
c = 16.381 (2) Å
β = 90.216 (6)°
V = 2645.3 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.89 mm^{-1}
T = 173.0 (1) K
0.15 × 0.15 × 0.07 mm

Data collection

Bruker X8 APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.701, T_{max} = 0.940
41680 measured reflections
12665 independent reflections
8610 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.080
S = 0.98
12665 reflections
668 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983), 6047 Friedel pairs
Flack parameter: 0.04 (4)

Table 1
Selected geometric parameters (Å, °).

C57—Rh1	1.803 (13)	P1—Rh1	2.3161 (11)
Cl1—Rh1	2.386 (3)	P2—Rh1	2.3207 (11)
C58—Rh2	1.770 (17)	P3—Rh2	2.3154 (11)
Cl2—Rh2	2.409 (4)	P4—Rh2	2.3132 (11)
C57—Rh1—P1	89.8 (4)	C58—Rh2—P4	91.4 (5)
C57—Rh1—P2	89.8 (4)	C58—Rh2—P3	89.2 (5)
P1—Rh1—P2	178.85 (7)	P4—Rh2—P3	179.25 (7)
C57—Rh1—Cl1	178.9 (4)	C58—Rh2—Cl2	177.0 (5)
P1—Rh1—Cl1	89.65 (9)	P4—Rh2—Cl2	89.25 (12)
P2—Rh1—Cl1	90.70 (9)	P3—Rh2—Cl2	90.22 (11)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C22—H22···O2^{i}	0.95	2.64	3.424 (18)	140
C48—H48···O1B^{ii}	0.95	2.68	3.51 (3)	145
C4—H4···O1B^{iii}	0.95	2.71	3.51 (3)	142

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+2$; (ii) $-x+2, y+\frac{1}{2}, -z+2$; (iii) $-x+2, y-\frac{1}{2}, -z+2$.

Data collection: *SAINT* (Bruker, 1997); cell refinement: *SAINT*; data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2391).

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trans-Carbonylchloridobis(ethyldiphenylphosphine-κP)rhodium(I)

Fabio Lorenzini, Brian O. Patrick and Brian R. James

S1. Comment

We have recently reported the syntheses of water-soluble Rh^{I}—THP complexes (THP is tris(hydroxymethyl)phosphine, $P(CH_2OH)_3$) (Lorenzini *et al.*, 2007*a*). During a subsequent study of the general reactivity of such complexes with other potential ligands, we discovered a remarkable reaction of RhCl(cod)(THP), where cod = 1,5-cyclooctadiene, with several PRR'_2 phosphines (R = or ≠ R'), that generates, concomitantly with $R'H$, the phosphine-phosphinite derivatives $RhCl(PRR'_2)[P,P—R'(R)POCH_2P(CH_2OH)_2]$ in two isomeric *cis*- and *trans*-forms (*cis* and *trans* refer to the disposition of the P-atoms with the R and R' substituents) (Lorenzini *et al.*, 2007*b*). Such reactions, when investigated under a hydrogen atmosphere, led to the serendipitous isolation of the dihydrido complexes *cis*,*mer*-$Rh(H)_2Cl(PRR'_2)_3$, where R = Me, R' = Ph, or R = Cy, R' = Ph (Lorenzini *et al.*, 2007*c*). $^{31}P\{^1H\}$ NMR data suggested the presence of traces of *trans*-$RhCl(CO)(PRR'_2)_2$ in some of the isolated $RhCl(PRR'_2)[P,P—R'(R)POCH_2P(CH_2OH)_2]$ complexes and in the *in situ* preparative solutions of the phosphine-phosphinite and dihydrido species (Lorenzini *et al.*, 2007*b*). The carbonyl ligand is thought to arise *via* decarbonylation of formaldehyde which can be readily formed from transition metal-THP species (Higham *et al.*, 2004; Hoye *et al.*, 1993); the Wilkinson-type complex such as $RhCl(PPh_3)_3$ is well known to decarbonylate aldehydes with formation of *trans*-$RhCl(CO)(PPh_3)_2$ (Beck *et al.*, 1999). The suggested formation of *trans*-$RhCl(CO)(PRR'_2)_2$ has now been confirmed by X-ray structural analysis of a single-crystal of *trans*-$RhCl(CO)(PEtPh_2)_2$ that was precipitated in trace yield during the reaction of RhCl(cod)(THP) with $PEtPh_2$, under a hydrogen atmosphere.

The complex *trans*-$RhCl(CO)(PPh_3)_2$ was first reported 50 years ago (Vallarino, 1957), but it was not until the Ir analogue (Vaska's compound) was synthesized (Vaska & Di Luzio, 1961) and shown to oxidatively add H_2 and other small molecules (Vaska & Di Luzio, 1962) that interest in such d^8 square-planar molecules intensified. According to the Cambridge Crystallography Data Base, there have been 125 crystallographically characterized complexes of the type *trans*-$RhCl(CO)(P\text{-phosphine})_2$, where $(P\text{-phosphine})_2$ represents two monodentate ligands or one bidentate phosphine ligand but there are none containing $PEtPh_2$. Indeed, in spite of the vast literature on the chemistry of Rh-phosphine complexes, we can find no other example of any isolated Rh-complex containing $PEtPh_2$, although an *in situ* $RhCl/PEtPh_2$ species has been noted (O′Connor & Wilkinson, 1969).

S2. Experimental

General. The RhCl(cod)(THP) complex was synthesized by our recently reported method; (Lorenzini *et al.*, 2007*a*) and $PEtPh_2$ was used as received from Strem Chemicals. The Rh-phosphine reaction was carried out under Ar or H_2 using standard Schlenk techniques. Acetone-d_6 and CD_3OD (Cambridge Isotope Laboratory) were used as received. $^{31}P\{^1H\}$-NMR spectra were measured in acetone-d_6 and CD_3OD at room temperature (~300 K) on a Bruker AV400 spectrometer. External 85% aq H_3PO_4 were used as references (d = doublet, m = multiplet).

Trans-$RhCl(CO)(PEtPh_2)_2$. Addition of $PEtPh_2$ (12 μL, 0.057 mmol) in acetone-d_6 (0.3 ml) to a yellow CD_3OD solution (0.3 ml) of RhCl(cod)(THP) (10 mg, 0.026 mmol) at room temperature under Ar results in the immediate formation of a

brown solution. The Ar is then replaced by H_2 and the vessel shaken, this resulting in a yellow solution. Over 12 h, a minute quantity of X-ray quality, yellow prism crystals of *trans*-RhCl(CO)($PEtPh_2$)$_2$ deposit from the solution; the $^{31}P\{^1H\}$ of the yellow solution shows the doublet resonance of the title compound (δ 27.49, d, J_{PRh} = 123.4 Hz) and also resonances at δ 36.64 (dd, 2P, J_{PRh} = 112.0, J_{PP} = 21.0 Hz, *trans*-P), and 18.29 (m, 1P, P-*trans* to Cl) thought to be due to $RhCl(PEtPh_2)_3$.

S3. Refinement

The material crystallizes with two molecules in the asymmetric unit. In each molecule the Cl and CO ligands are positionally disordered. Each was modelled such that the sum of the ligands at each coordination site was 1.

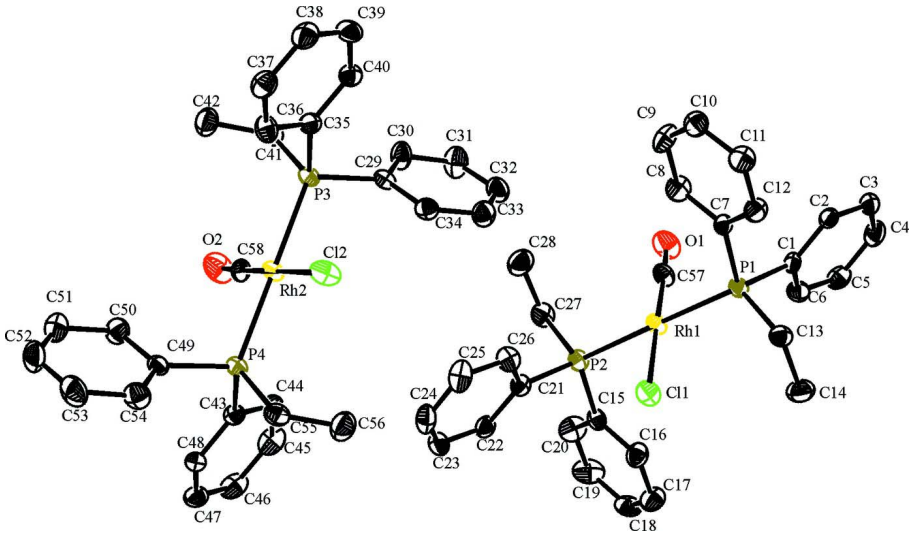

Figure 1

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trans-Carbonylchloridobis(ethyldiphenylphosphine-κP)rhodium(I)

Crystal data

$[RhCl(C_{14}H_{15}P)_2(CO)]$
M_r = 594.83
Monoclinic, $P2_1$
a = 9.8557 (14) Å
b = 16.385 (2) Å
c = 16.381 (2) Å
β = 90.216 (6)°
V = 2645.3 (6) Å^3
Z = 4
$F(000)$ = 1216
D_x = 1.494 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6687 reflections
θ = 2.4–27.8°
μ = 0.89 mm^{-1}
T = 173 K
Prism, yellow
0.15 × 0.15 × 0.07 mm

Data collection

Bruker X8 APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
area–detector scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.701, T_{max} = 0.940
41680 measured reflections
12665 independent reflections
8610 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 28.0°, θ_{min} = 1.8°
h = −12→12
k = −21→21
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.080$
$S = 0.98$
12665 reflections
668 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}
Absolute structure: Flack (1983), 6047 Friedel pairs
Absolute structure parameter: 0.04 (4)

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}	Occ. (<1)
C1	0.9538 (4)	0.4119 (3)	0.9327 (3)	0.0217 (10)	
C2	0.9587 (4)	0.4211 (3)	0.8491 (3)	0.0229 (10)	
H2	0.9777	0.4729	0.8258	0.027*	
C3	0.9356 (4)	0.3539 (3)	0.7992 (3)	0.0286 (10)	
H3	0.9371	0.3607	0.7417	0.034*	
C4	0.9107 (5)	0.2785 (3)	0.8311 (3)	0.0337 (13)	
H4	0.8969	0.2331	0.7961	0.040*	
C5	0.9058 (5)	0.2687 (3)	0.9160 (4)	0.0306 (13)	
H5	0.8886	0.2167	0.9392	0.037*	
C6	0.9264 (5)	0.3359 (3)	0.9653 (3)	0.0288 (11)	
H6	0.9216	0.3298	1.0228	0.035*	
C7	0.9578 (5)	0.5884 (3)	0.9429 (3)	0.0201 (11)	
C8	0.8304 (5)	0.6227 (3)	0.9481 (3)	0.0318 (13)	
H8	0.7639	0.5988	0.9824	0.038*	
C9	0.7990 (5)	0.6921 (3)	0.9032 (3)	0.0381 (13)	
H9	0.7106	0.7150	0.9062	0.046*	
C10	0.8947 (6)	0.7274 (3)	0.8551 (4)	0.0306 (14)	
H10	0.8739	0.7759	0.8258	0.037*	
C11	1.0193 (5)	0.6935 (3)	0.8489 (3)	0.0327 (12)	
H11	1.0847	0.7177	0.8139	0.039*	
C12	1.0527 (5)	0.6247 (3)	0.8924 (3)	0.0285 (10)	
H12	1.1411	0.6020	0.8879	0.034*	
C13	1.1777 (4)	0.4925 (3)	1.0074 (2)	0.0253 (9)	

H13A	1.2141	0.4929	0.9512	0.030*
H13B	1.2108	0.5423	1.0353	0.030*
C14	1.2332 (5)	0.4181 (3)	1.0520 (3)	0.0389 (12)
H14A	1.1982	0.4171	1.1078	0.058*
H14B	1.3325	0.4208	1.0534	0.058*
H14C	1.2048	0.3684	1.0233	0.058*
C15	0.8052 (5)	0.4018 (3)	1.3072 (3)	0.0229 (11)
C16	0.9351 (5)	0.3710 (3)	1.3029 (3)	0.0318 (13)
H16	1.0003	0.3982	1.2702	0.038*
C17	0.9731 (5)	0.3013 (3)	1.3452 (3)	0.0377 (13)
H17	1.0636	0.2817	1.3423	0.045*
C18	0.8783 (6)	0.2608 (4)	1.3914 (4)	0.0361 (14)
H18	0.9026	0.2123	1.4196	0.043*
C19	0.7478 (5)	0.2909 (3)	1.3967 (3)	0.0430 (14)
H19	0.6826	0.2632	1.4290	0.052*
C20	0.7116 (5)	0.3606 (3)	1.3554 (3)	0.0379 (12)
H20	0.6216	0.3808	1.3597	0.045*
C21	0.7961 (4)	0.5771 (3)	1.3191 (3)	0.0225 (10)
C22	0.7836 (4)	0.5671 (3)	1.4027 (3)	0.0261 (10)
H22	0.7622	0.5150	1.4245	0.031*
C23	0.8021 (5)	0.6328 (3)	1.4547 (3)	0.0333 (12)
H23	0.7933	0.6254	1.5119	0.040*
C24	0.8332 (5)	0.7093 (3)	1.4237 (3)	0.0349 (13)
H24	0.8478	0.7540	1.4596	0.042*
C25	0.8427 (5)	0.7200 (3)	1.3417 (4)	0.0361 (14)
H25	0.8614	0.7727	1.3204	0.043*
C26	0.8254 (5)	0.6549 (3)	1.2888 (3)	0.0296 (11)
H26	0.8334	0.6631	1.2316	0.036*
C27	0.5785 (4)	0.4937 (3)	1.2440 (3)	0.0316 (10)
H27A	0.5477	0.4440	1.2150	0.038*
H27B	0.5423	0.4914	1.3002	0.038*
C28	0.5200 (5)	0.5684 (3)	1.2010 (3)	0.0428 (13)
H28A	0.5491	0.6179	1.2297	0.064*
H28B	0.4208	0.5652	1.2010	0.064*
H28C	0.5527	0.5700	1.1445	0.064*
C29	0.5462 (5)	0.9084 (3)	0.1954 (3)	0.0207 (11)
C30	0.4458 (5)	0.8558 (3)	0.1673 (3)	0.0323 (11)
H30	0.3528	0.8693	0.1746	0.039*
C31	0.4809 (5)	0.7846 (3)	0.1291 (3)	0.0377 (13)
H31	0.4116	0.7479	0.1124	0.045*
C32	0.6137 (6)	0.7653 (4)	0.1143 (4)	0.0317 (14)
H32	0.6365	0.7166	0.0860	0.038*
C33	0.7145 (5)	0.8179 (3)	0.1414 (3)	0.0317 (11)
H33	0.8072	0.8052	0.1320	0.038*
C34	0.6804 (5)	0.8888 (3)	0.1821 (3)	0.0249 (11)
H34	0.7499	0.9244	0.2009	0.030*
C35	0.5486 (4)	1.0840 (3)	0.1819 (3)	0.0228 (10)
C36	0.5895 (5)	1.1597 (3)	0.2134 (3)	0.0290 (11)

H36	0.6007	1.1668	0.2706	0.035*	
C37	0.6134 (5)	1.2244 (3)	0.1605 (4)	0.0308 (13)	
H37	0.6409	1.2757	0.1819	0.037*	
C38	0.5980 (5)	1.2152 (3)	0.0787 (3)	0.0335 (13)	
H38	0.6141	1.2601	0.0434	0.040*	
C39	0.5591 (5)	1.1409 (3)	0.0463 (3)	0.0316 (11)	
H39	0.5500	1.1345	−0.0111	0.038*	
C40	0.5333 (4)	1.0753 (3)	0.0982 (3)	0.0259 (10)	
H40	0.5051	1.0244	0.0762	0.031*	
C41	0.3228 (4)	1.0043 (3)	0.2550 (2)	0.0264 (9)	
H41A	0.2872	1.0006	0.1985	0.032*	
H41B	0.2894	0.9562	0.2855	0.032*	
C42	0.2677 (5)	1.0820 (3)	0.2950 (3)	0.0372 (12)	
H42A	0.3008	1.0854	0.3514	0.056*	
H42B	0.1683	1.0805	0.2949	0.056*	
H42C	0.2987	1.1298	0.2644	0.056*	
C43	0.6994 (4)	0.9272 (3)	0.5727 (3)	0.0225 (10)	
C44	0.6515 (4)	0.8529 (3)	0.5463 (3)	0.0265 (11)	
H44	0.6356	0.8441	0.4898	0.032*	
C45	0.6264 (5)	0.7911 (3)	0.6014 (4)	0.0368 (15)	
H45	0.5937	0.7398	0.5828	0.044*	
C46	0.6488 (5)	0.8042 (3)	0.6836 (3)	0.0356 (13)	
H46	0.6312	0.7619	0.7218	0.043*	
C47	0.6962 (5)	0.8777 (3)	0.7100 (3)	0.0334 (12)	
H47	0.7106	0.8866	0.7666	0.040*	
C48	0.7234 (4)	0.9395 (3)	0.6551 (3)	0.0254 (10)	
H48	0.7584	0.9902	0.6738	0.030*	
C49	0.7068 (5)	1.1020 (3)	0.5537 (3)	0.0213 (11)	
C50	0.5730 (5)	1.1252 (3)	0.5646 (3)	0.0305 (13)	
H50	0.5021	1.0916	0.5440	0.037*	
C51	0.5414 (5)	1.1965 (3)	0.6052 (3)	0.0397 (13)	
H51	0.4492	1.2108	0.6140	0.048*	
C52	0.6422 (6)	1.2462 (4)	0.6325 (4)	0.0405 (16)	
H52	0.6202	1.2958	0.6595	0.049*	
C53	0.7755 (5)	1.2252 (3)	0.6212 (3)	0.0404 (13)	
H53	0.8457	1.2604	0.6398	0.049*	
C54	0.8080 (5)	1.1519 (3)	0.5823 (3)	0.0321 (11)	
H54	0.9003	1.1366	0.5758	0.039*	
C55	0.9249 (4)	1.0010 (3)	0.4947 (2)	0.0272 (9)	
H55A	0.9594	1.0481	0.4631	0.033*	
H55B	0.9612	1.0057	0.5509	0.033*	
C56	0.9788 (5)	0.9231 (3)	0.4568 (3)	0.0389 (13)	
H56A	0.9535	0.8765	0.4910	0.058*	
H56B	1.0779	0.9263	0.4530	0.058*	
H56C	0.9399	0.9163	0.4021	0.058*	
O1	0.6403 (12)	0.4282 (9)	1.0455 (9)	0.042 (3)	0.690 (16)
C57	0.7319 (13)	0.4523 (8)	1.0755 (8)	0.026 (2)	0.690 (16)
Cl1	1.0740 (4)	0.5520 (2)	1.1907 (2)	0.0325 (13)	0.690 (16)

O2	0.3780 (16)	0.9494 (11)	0.4549 (11)	0.046 (4)	0.505 (16)
C58	0.4754 (16)	0.9675 (10)	0.4244 (9)	0.029 (3)	0.505 (16)
Cl2	0.8281 (4)	1.0452 (3)	0.3070 (3)	0.0330 (16)	0.505 (16)
O1B	1.118 (2)	0.5677 (18)	1.2021 (16)	0.036 (6)	0.310 (16)
C57B	1.017 (3)	0.5407 (15)	1.1698 (14)	0.024 (5)	0.310 (16)
Cl1B	0.6789 (8)	0.4422 (6)	1.0585 (5)	0.029 (2)	0.310 (16)
O2B	0.8740 (14)	1.0596 (10)	0.2968 (9)	0.044 (3)	0.495 (16)
C58B	0.7709 (15)	1.0374 (7)	0.3261 (8)	0.028 (3)*	0.495 (16)
Cl2B	0.4212 (5)	0.9610 (3)	0.4431 (3)	0.0271 (16)	0.495 (16)
P1	0.99277 (10)	0.49628 (8)	1.00219 (6)	0.0213 (2)	
P2	0.76358 (10)	0.49333 (8)	1.24884 (6)	0.0232 (2)	
P3	0.50860 (10)	1.00148 (8)	0.25227 (6)	0.0206 (2)	
P4	0.74016 (10)	1.00706 (8)	0.49855 (6)	0.0207 (2)	
Rh1	0.87809 (4)	0.49622 (3)	1.12535 (3)	0.02214 (9)	
Rh2	0.62381 (4)	1.00347 (3)	0.37570 (3)	0.02055 (8)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.020 (2)	0.023 (2)	0.022 (2)	0.0041 (18)	0.0033 (18)	−0.0033 (19)
C2	0.021 (2)	0.023 (2)	0.024 (2)	0.0045 (18)	0.0029 (18)	0.0027 (18)
C3	0.028 (2)	0.033 (3)	0.025 (3)	0.006 (2)	−0.0021 (19)	−0.007 (2)
C4	0.032 (3)	0.028 (3)	0.041 (3)	0.005 (2)	−0.001 (2)	−0.011 (2)
C5	0.031 (3)	0.021 (3)	0.040 (3)	0.002 (2)	0.002 (2)	0.007 (2)
C6	0.035 (3)	0.026 (3)	0.025 (3)	0.003 (2)	0.002 (2)	0.005 (2)
C7	0.022 (2)	0.018 (2)	0.021 (3)	0.0014 (18)	0.0001 (19)	−0.0026 (19)
C8	0.031 (3)	0.031 (3)	0.034 (3)	−0.003 (2)	0.009 (2)	0.008 (2)
C9	0.026 (3)	0.037 (3)	0.051 (4)	0.010 (2)	0.005 (2)	0.000 (3)
C10	0.038 (3)	0.022 (3)	0.032 (3)	0.001 (2)	0.001 (2)	0.000 (2)
C11	0.035 (3)	0.029 (3)	0.034 (3)	−0.002 (2)	0.005 (2)	0.007 (2)
C12	0.026 (2)	0.030 (2)	0.029 (3)	0.002 (2)	0.007 (2)	0.007 (2)
C13	0.023 (2)	0.029 (2)	0.024 (2)	−0.002 (2)	0.0001 (16)	0.004 (2)
C14	0.036 (3)	0.044 (3)	0.036 (3)	0.007 (2)	−0.003 (2)	0.011 (2)
C15	0.028 (3)	0.020 (2)	0.021 (3)	−0.0035 (19)	0.0034 (19)	−0.0016 (19)
C16	0.032 (3)	0.030 (3)	0.034 (3)	0.003 (2)	0.007 (2)	0.003 (2)
C17	0.039 (3)	0.038 (3)	0.036 (3)	0.009 (2)	0.008 (2)	0.015 (2)
C18	0.054 (4)	0.025 (3)	0.029 (3)	0.000 (2)	−0.009 (3)	0.009 (2)
C19	0.043 (3)	0.045 (3)	0.041 (3)	−0.013 (3)	0.002 (2)	0.023 (3)
C20	0.030 (3)	0.039 (3)	0.045 (3)	−0.007 (2)	0.005 (2)	0.011 (2)
C21	0.019 (2)	0.024 (2)	0.024 (2)	−0.0016 (18)	0.0049 (18)	0.0018 (18)
C22	0.022 (2)	0.029 (2)	0.027 (2)	0.0041 (19)	0.0048 (18)	0.002 (2)
C23	0.031 (3)	0.045 (3)	0.024 (3)	0.006 (2)	0.003 (2)	−0.005 (2)
C24	0.031 (3)	0.032 (3)	0.042 (3)	0.001 (2)	0.006 (2)	−0.014 (2)
C25	0.034 (3)	0.025 (3)	0.049 (4)	−0.006 (2)	0.014 (3)	−0.004 (2)
C26	0.031 (3)	0.029 (3)	0.029 (3)	−0.005 (2)	0.004 (2)	0.002 (2)
C27	0.025 (2)	0.039 (3)	0.030 (2)	−0.005 (2)	0.0068 (17)	0.002 (2)
C28	0.031 (3)	0.050 (3)	0.048 (3)	0.007 (2)	0.004 (2)	0.003 (3)
C29	0.022 (3)	0.024 (3)	0.016 (3)	−0.005 (2)	−0.0011 (19)	0.000 (2)

C30	0.024 (2)	0.033 (3)	0.039 (3)	−0.002 (2)	0.001 (2)	−0.015 (2)
C31	0.033 (3)	0.031 (3)	0.049 (4)	−0.010 (2)	0.004 (2)	−0.014 (2)
C32	0.039 (3)	0.029 (3)	0.028 (3)	−0.001 (2)	−0.002 (2)	−0.007 (2)
C33	0.025 (3)	0.037 (3)	0.034 (3)	0.000 (2)	0.002 (2)	−0.004 (2)
C34	0.022 (2)	0.026 (3)	0.026 (3)	−0.004 (2)	−0.004 (2)	−0.002 (2)
C35	0.020 (2)	0.027 (2)	0.021 (2)	0.0020 (19)	0.0016 (18)	0.0037 (19)
C36	0.034 (3)	0.024 (2)	0.029 (3)	−0.004 (2)	0.002 (2)	−0.006 (2)
C37	0.028 (3)	0.024 (3)	0.040 (3)	0.000 (2)	−0.001 (2)	−0.001 (2)
C38	0.040 (3)	0.026 (3)	0.034 (3)	0.005 (2)	0.008 (2)	0.010 (2)
C39	0.034 (3)	0.041 (3)	0.020 (2)	0.005 (2)	0.0040 (19)	0.009 (2)
C40	0.025 (2)	0.026 (2)	0.026 (2)	0.0012 (18)	−0.0019 (18)	−0.0007 (19)
C41	0.021 (2)	0.031 (3)	0.027 (2)	−0.004 (2)	−0.0003 (16)	−0.001 (2)
C42	0.032 (3)	0.037 (3)	0.042 (3)	0.007 (2)	0.003 (2)	−0.007 (2)
C43	0.021 (2)	0.022 (2)	0.024 (2)	0.0003 (18)	−0.0012 (18)	0.0003 (18)
C44	0.028 (3)	0.026 (2)	0.025 (3)	0.005 (2)	−0.001 (2)	0.001 (2)
C45	0.033 (3)	0.025 (3)	0.053 (4)	−0.003 (2)	0.005 (3)	0.007 (3)
C46	0.033 (3)	0.035 (3)	0.039 (3)	0.004 (2)	0.010 (2)	0.019 (2)
C47	0.032 (3)	0.047 (3)	0.022 (3)	0.013 (2)	0.004 (2)	0.008 (2)
C48	0.028 (2)	0.027 (2)	0.021 (2)	0.0058 (19)	−0.0035 (18)	−0.0013 (19)
C49	0.029 (3)	0.018 (2)	0.017 (3)	−0.0006 (19)	−0.0038 (19)	−0.0008 (18)
C50	0.032 (3)	0.023 (3)	0.036 (3)	−0.002 (2)	−0.003 (2)	−0.005 (2)
C51	0.039 (3)	0.040 (3)	0.040 (3)	0.010 (2)	0.002 (3)	−0.008 (3)
C52	0.057 (4)	0.026 (3)	0.038 (4)	0.008 (3)	0.003 (3)	−0.009 (3)
C53	0.049 (3)	0.034 (3)	0.038 (3)	−0.008 (3)	−0.006 (3)	−0.012 (2)
C54	0.029 (3)	0.034 (3)	0.034 (3)	−0.005 (2)	−0.003 (2)	−0.003 (2)
C55	0.025 (2)	0.031 (3)	0.026 (2)	−0.004 (2)	−0.0040 (16)	−0.001 (2)
C56	0.031 (3)	0.041 (3)	0.045 (3)	0.006 (2)	0.003 (2)	−0.005 (3)
O1	0.033 (7)	0.056 (6)	0.038 (6)	−0.015 (5)	−0.003 (4)	−0.009 (4)
C57	0.025 (7)	0.031 (5)	0.021 (5)	−0.007 (5)	0.003 (5)	−0.001 (4)
Cl1	0.032 (3)	0.037 (2)	0.028 (2)	−0.004 (2)	0.0013 (19)	−0.0021 (15)
O2	0.040 (9)	0.064 (8)	0.033 (7)	−0.009 (6)	0.011 (6)	0.001 (5)
C58	0.025 (8)	0.040 (7)	0.020 (6)	0.012 (6)	0.009 (5)	0.000 (5)
Cl2	0.027 (4)	0.045 (2)	0.027 (2)	−0.0107 (19)	−0.001 (2)	0.0060 (14)
O1B	0.022 (12)	0.041 (13)	0.046 (11)	−0.005 (8)	−0.015 (8)	0.002 (8)
C57B	0.032 (14)	0.027 (10)	0.014 (10)	0.006 (10)	0.003 (9)	−0.007 (8)
Cl1B	0.017 (6)	0.045 (4)	0.026 (5)	−0.016 (4)	−0.006 (4)	−0.008 (3)
O2B	0.024 (7)	0.060 (7)	0.048 (7)	−0.019 (5)	0.004 (5)	0.005 (5)
Cl2B	0.022 (4)	0.038 (2)	0.022 (3)	−0.003 (2)	0.004 (2)	0.0006 (17)
P1	0.0240 (5)	0.0224 (6)	0.0175 (5)	0.0000 (5)	0.0027 (4)	0.0026 (5)
P2	0.0233 (5)	0.0245 (6)	0.0219 (6)	−0.0033 (5)	0.0042 (4)	0.0027 (5)
P3	0.0218 (5)	0.0226 (6)	0.0175 (5)	−0.0030 (5)	−0.0024 (4)	−0.0018 (5)
P4	0.0224 (5)	0.0219 (6)	0.0179 (5)	−0.0024 (5)	−0.0023 (4)	−0.0016 (5)
Rh1	0.02361 (14)	0.0258 (2)	0.01709 (13)	−0.00473 (15)	0.00288 (10)	0.00149 (14)
Rh2	0.02122 (13)	0.0247 (2)	0.01573 (12)	−0.00439 (14)	−0.00130 (9)	−0.00039 (13)

Geometric parameters (Å, º)

C1—C2	1.379 (6)	C32—H32	0.9500
C1—C6	1.381 (6)	C33—C34	1.382 (7)
C1—P1	1.831 (4)	C33—H33	0.9500
C2—C3	1.388 (6)	C34—H34	0.9500
C2—H2	0.9500	C35—C40	1.385 (6)
C3—C4	1.363 (6)	C35—C36	1.403 (6)
C3—H3	0.9500	C35—P3	1.821 (4)
C4—C5	1.400 (8)	C36—C37	1.390 (7)
C4—H4	0.9500	C36—H36	0.9500
C5—C6	1.380 (7)	C37—C38	1.357 (8)
C5—H5	0.9500	C37—H37	0.9500
C6—H6	0.9500	C38—C39	1.381 (7)
C7—C8	1.379 (6)	C38—H38	0.9500
C7—C12	1.385 (6)	C39—C40	1.395 (6)
C7—P1	1.827 (5)	C39—H39	0.9500
C8—C9	1.388 (7)	C40—H40	0.9500
C8—H8	0.9500	C41—C42	1.533 (6)
C9—C10	1.360 (7)	C41—P3	1.832 (4)
C9—H9	0.9500	C41—H41A	0.9900
C10—C11	1.352 (7)	C41—H41B	0.9900
C10—H10	0.9500	C42—H42A	0.9800
C11—C12	1.374 (6)	C42—H42B	0.9800
C11—H11	0.9500	C42—H42C	0.9800
C12—H12	0.9500	C43—C44	1.374 (6)
C13—C14	1.521 (6)	C43—C48	1.384 (6)
C13—P1	1.825 (4)	C43—P4	1.831 (4)
C13—H13A	0.9900	C44—C45	1.379 (7)
C13—H13B	0.9900	C44—H44	0.9500
C14—H14A	0.9800	C45—C46	1.381 (8)
C14—H14B	0.9800	C45—H45	0.9500
C14—H14C	0.9800	C46—C47	1.362 (7)
C15—C16	1.378 (7)	C46—H46	0.9500
C15—C20	1.392 (7)	C47—C48	1.381 (6)
C15—P2	1.824 (5)	C47—H47	0.9500
C16—C17	1.387 (7)	C48—H48	0.9500
C16—H16	0.9500	C49—C54	1.371 (6)
C17—C18	1.375 (7)	C49—C50	1.385 (7)
C17—H17	0.9500	C49—P4	1.829 (5)
C18—C19	1.380 (7)	C50—C51	1.380 (6)
C18—H18	0.9500	C50—H50	0.9500
C19—C20	1.374 (7)	C51—C52	1.359 (8)
C19—H19	0.9500	C51—H51	0.9500
C20—H20	0.9500	C52—C53	1.372 (7)
C21—C22	1.385 (6)	C52—H52	0.9500
C21—C26	1.399 (6)	C53—C54	1.397 (6)
C21—P2	1.818 (4)	C53—H53	0.9500

C22—C23	1.383 (6)	C54—H54	0.9500
C22—H22	0.9500	C55—C56	1.516 (6)
C23—C24	1.387 (7)	C55—P4	1.825 (4)
C23—H23	0.9500	C55—H55A	0.9900
C24—C25	1.358 (8)	C55—H55B	0.9900
C24—H24	0.9500	C56—H56A	0.9800
C25—C26	1.385 (7)	C56—H56B	0.9800
C25—H25	0.9500	C56—H56C	0.9800
C26—H26	0.9500	O1—C57	1.10 (2)
C27—C28	1.524 (6)	C57—Rh1	1.803 (13)
C27—P2	1.825 (4)	Cl1—Rh1	2.386 (3)
C27—H27A	0.9900	O2—C58	1.12 (3)
C27—H27B	0.9900	C58—Rh2	1.770 (17)
C28—H28A	0.9800	Cl2—Rh2	2.409 (4)
C28—H28B	0.9800	O1B—C57B	1.21 (4)
C28—H28C	0.9800	C57B—Rh1	1.71 (3)
C29—C34	1.379 (6)	Cl1B—Rh1	2.412 (6)
C29—C30	1.390 (6)	O2B—C58B	1.18 (3)
C29—P3	1.826 (5)	C58B—Rh2	1.755 (17)
C30—C31	1.369 (6)	Cl2B—Rh2	2.389 (4)
C30—H30	0.9500	P1—Rh1	2.3161 (11)
C31—C32	1.370 (7)	P2—Rh1	2.3207 (11)
C31—H31	0.9500	P3—Rh2	2.3154 (11)
C32—C33	1.388 (7)	P4—Rh2	2.3132 (11)

C2—C1—C6	119.3 (4)	C39—C38—H38	119.8
C2—C1—P1	121.8 (3)	C38—C39—C40	119.7 (4)
C6—C1—P1	118.8 (3)	C38—C39—H39	120.1
C1—C2—C3	119.4 (4)	C40—C39—H39	120.1
C1—C2—H2	120.3	C35—C40—C39	120.3 (4)
C3—C2—H2	120.3	C35—C40—H40	119.8
C4—C3—C2	121.5 (5)	C39—C40—H40	119.8
C4—C3—H3	119.3	C42—C41—P3	112.7 (3)
C2—C3—H3	119.3	C42—C41—H41A	109.0
C3—C4—C5	119.4 (5)	P3—C41—H41A	109.0
C3—C4—H4	120.3	C42—C41—H41B	109.0
C5—C4—H4	120.3	P3—C41—H41B	109.0
C6—C5—C4	118.9 (5)	H41A—C41—H41B	107.8
C6—C5—H5	120.5	C41—C42—H42A	109.5
C4—C5—H5	120.5	C41—C42—H42B	109.5
C5—C6—C1	121.4 (4)	H42A—C42—H42B	109.5
C5—C6—H6	119.3	C41—C42—H42C	109.5
C1—C6—H6	119.3	H42A—C42—H42C	109.5
C8—C7—C12	118.6 (4)	H42B—C42—H42C	109.5
C8—C7—P1	118.3 (4)	C44—C43—C48	119.5 (4)
C12—C7—P1	123.1 (4)	C44—C43—P4	120.0 (3)
C7—C8—C9	120.2 (4)	C48—C43—P4	120.3 (3)
C7—C8—H8	119.9	C43—C44—C45	120.5 (5)

C9—C8—H8	119.9	C43—C44—H44	119.8
C10—C9—C8	120.1 (5)	C45—C44—H44	119.8
C10—C9—H9	120.0	C44—C45—C46	119.7 (5)
C8—C9—H9	120.0	C44—C45—H45	120.2
C11—C10—C9	120.0 (5)	C46—C45—H45	120.2
C11—C10—H10	120.0	C47—C46—C45	120.0 (5)
C9—C10—H10	120.0	C47—C46—H46	120.0
C10—C11—C12	121.0 (5)	C45—C46—H46	120.0
C10—C11—H11	119.5	C46—C47—C48	120.6 (5)
C12—C11—H11	119.5	C46—C47—H47	119.7
C11—C12—C7	120.1 (4)	C48—C47—H47	119.7
C11—C12—H12	120.0	C47—C48—C43	119.7 (4)
C7—C12—H12	120.0	C47—C48—H48	120.2
C14—C13—P1	114.0 (3)	C43—C48—H48	120.2
C14—C13—H13A	108.7	C54—C49—C50	118.9 (4)
P1—C13—H13A	108.7	C54—C49—P4	123.0 (4)
C14—C13—H13B	108.7	C50—C49—P4	118.0 (4)
P1—C13—H13B	108.7	C51—C50—C49	120.8 (5)
H13A—C13—H13B	107.6	C51—C50—H50	119.6
C13—C14—H14A	109.5	C49—C50—H50	119.6
C13—C14—H14B	109.5	C52—C51—C50	120.0 (5)
H14A—C14—H14B	109.5	C52—C51—H51	120.0
C13—C14—H14C	109.5	C50—C51—H51	120.0
H14A—C14—H14C	109.5	C51—C52—C53	120.3 (5)
H14B—C14—H14C	109.5	C51—C52—H52	119.9
C16—C15—C20	118.0 (5)	C53—C52—H52	119.9
C16—C15—P2	118.8 (4)	C52—C53—C54	119.9 (5)
C20—C15—P2	123.2 (4)	C52—C53—H53	120.0
C15—C16—C17	121.7 (5)	C54—C53—H53	120.0
C15—C16—H16	119.1	C49—C54—C53	120.1 (5)
C17—C16—H16	119.1	C49—C54—H54	120.0
C18—C17—C16	119.3 (5)	C53—C54—H54	120.0
C18—C17—H17	120.3	C56—C55—P4	114.3 (3)
C16—C17—H17	120.3	C56—C55—H55A	108.7
C17—C18—C19	119.9 (5)	P4—C55—H55A	108.7
C17—C18—H18	120.1	C56—C55—H55B	108.7
C19—C18—H18	120.1	P4—C55—H55B	108.7
C20—C19—C18	120.4 (5)	H55A—C55—H55B	107.6
C20—C19—H19	119.8	C55—C56—H56A	109.5
C18—C19—H19	119.8	C55—C56—H56B	109.5
C19—C20—C15	120.8 (5)	H56A—C56—H56B	109.5
C19—C20—H20	119.6	C55—C56—H56C	109.5
C15—C20—H20	119.6	H56A—C56—H56C	109.5
C22—C21—C26	118.5 (4)	H56B—C56—H56C	109.5
C22—C21—P2	121.4 (3)	O1—C57—Rh1	177.3 (16)
C26—C21—P2	119.9 (4)	O2—C58—Rh2	175.7 (19)
C23—C22—C21	120.3 (4)	O1B—C57B—Rh1	176 (3)
C23—C22—H22	119.8	O2B—C58B—Rh2	176.1 (14)

C21—C22—H22	119.8	C13—P1—C7	103.8 (2)
C22—C23—C24	120.5 (4)	C13—P1—C1	102.2 (2)
C22—C23—H23	119.8	C7—P1—C1	104.76 (19)
C24—C23—H23	119.8	C13—P1—Rh1	116.71 (13)
C25—C24—C23	119.6 (5)	C7—P1—Rh1	111.83 (16)
C25—C24—H24	120.2	C1—P1—Rh1	116.06 (15)
C23—C24—H24	120.2	C21—P2—C15	104.4 (2)
C24—C25—C26	120.7 (5)	C21—P2—C27	101.5 (2)
C24—C25—H25	119.6	C15—P2—C27	104.4 (2)
C26—C25—H25	119.6	C21—P2—Rh1	116.82 (14)
C25—C26—C21	120.3 (5)	C15—P2—Rh1	111.38 (17)
C25—C26—H26	119.8	C27—P2—Rh1	116.82 (14)
C21—C26—H26	119.8	C35—P3—C29	104.62 (19)
C28—C27—P2	113.5 (3)	C35—P3—C41	102.4 (2)
C28—C27—H27A	108.9	C29—P3—C41	103.8 (2)
P2—C27—H27A	108.9	C35—P3—Rh2	115.85 (15)
C28—C27—H27B	108.9	C29—P3—Rh2	110.93 (16)
P2—C27—H27B	108.9	C41—P3—Rh2	117.74 (13)
H27A—C27—H27B	107.7	C55—P4—C49	104.2 (2)
C27—C28—H28A	109.5	C55—P4—C43	101.9 (2)
C27—C28—H28B	109.5	C49—P4—C43	103.9 (2)
H28A—C28—H28B	109.5	C55—P4—Rh2	117.37 (13)
C27—C28—H28C	109.5	C49—P4—Rh2	111.21 (17)
H28A—C28—H28C	109.5	C43—P4—Rh2	116.70 (15)
H28B—C28—H28C	109.5	C57B—Rh1—C57	177.8 (11)
C34—C29—C30	119.1 (4)	C57B—Rh1—P1	88.7 (8)
C34—C29—P3	118.2 (3)	C57—Rh1—P1	89.8 (4)
C30—C29—P3	122.7 (4)	C57B—Rh1—P2	91.7 (8)
C31—C30—C29	119.9 (5)	C57—Rh1—P2	89.8 (4)
C31—C30—H30	120.0	P1—Rh1—P2	178.85 (7)
C29—C30—H30	120.0	C57B—Rh1—Cl1	2.8 (8)
C30—C31—C32	121.4 (5)	C57—Rh1—Cl1	178.9 (4)
C30—C31—H31	119.3	P1—Rh1—Cl1	89.65 (9)
C32—C31—H31	119.3	P2—Rh1—Cl1	90.70 (9)
C31—C32—C33	118.9 (5)	C57B—Rh1—Cl1B	176.2 (9)
C31—C32—H32	120.6	C57—Rh1—Cl1B	2.0 (4)
C33—C32—H32	120.6	P1—Rh1—Cl1B	90.2 (2)
C34—C33—C32	120.1 (5)	P2—Rh1—Cl1B	89.5 (2)
C34—C33—H33	119.9	Cl1—Rh1—Cl1B	179.0 (3)
C32—C33—H33	119.9	C58B—Rh2—C58	178.8 (7)
C29—C34—C33	120.5 (4)	C58B—Rh2—P4	89.3 (4)
C29—C34—H34	119.8	C58—Rh2—P4	91.4 (5)
C33—C34—H34	119.8	C58B—Rh2—P3	90.2 (4)
C40—C35—C36	119.0 (4)	C58—Rh2—P3	89.2 (5)
C40—C35—P3	121.8 (3)	P4—Rh2—P3	179.25 (7)
C36—C35—P3	119.1 (3)	C58B—Rh2—Cl2B	178.4 (4)
C37—C36—C35	119.6 (5)	C58—Rh2—Cl2B	2.5 (5)
C37—C36—H36	120.2	P4—Rh2—Cl2B	91.03 (13)

C35—C36—H36	120.2	P3—Rh2—Cl2B	89.50 (13)
C38—C37—C36	120.8 (5)	C58B—Rh2—Cl2	2.0 (4)
C38—C37—H37	119.6	C58—Rh2—Cl2	177.0 (5)
C36—C37—H37	119.6	P4—Rh2—Cl2	89.25 (12)
C37—C38—C39	120.5 (5)	P3—Rh2—Cl2	90.22 (11)
C37—C38—H38	119.8	Cl2B—Rh2—Cl2	179.5 (2)

C6—C1—C2—C3	0.2 (6)	C16—C15—P2—C21	−91.8 (5)
P1—C1—C2—C3	176.4 (3)	C20—C15—P2—C21	89.1 (5)
C1—C2—C3—C4	−1.3 (7)	C16—C15—P2—C27	162.0 (4)
C2—C3—C4—C5	1.2 (7)	C20—C15—P2—C27	−17.0 (5)
C3—C4—C5—C6	0.0 (7)	C16—C15—P2—Rh1	35.1 (5)
C4—C5—C6—C1	−1.1 (7)	C20—C15—P2—Rh1	−144.0 (4)
C2—C1—C6—C5	1.0 (7)	C28—C27—P2—C21	68.7 (4)
P1—C1—C6—C5	−175.3 (4)	C28—C27—P2—C15	177.0 (3)
C12—C7—C8—C9	0.1 (8)	C28—C27—P2—Rh1	−59.5 (4)
P1—C7—C8—C9	−179.2 (4)	C40—C35—P3—C29	31.4 (4)
C7—C8—C9—C10	−1.2 (8)	C36—C35—P3—C29	−151.8 (4)
C8—C9—C10—C11	2.0 (9)	C40—C35—P3—C41	−76.6 (4)
C9—C10—C11—C12	−1.8 (9)	C36—C35—P3—C41	100.1 (4)
C10—C11—C12—C7	0.7 (8)	C40—C35—P3—Rh2	153.9 (3)
C8—C7—C12—C11	0.1 (7)	C36—C35—P3—Rh2	−29.4 (4)
P1—C7—C12—C11	179.4 (4)	C34—C29—P3—C35	72.5 (4)
C20—C15—C16—C17	−0.3 (8)	C30—C29—P3—C35	−109.3 (4)
P2—C15—C16—C17	−179.4 (4)	C34—C29—P3—C41	179.5 (4)
C15—C16—C17—C18	1.3 (9)	C30—C29—P3—C41	−2.3 (5)
C16—C17—C18—C19	−1.4 (9)	C34—C29—P3—Rh2	−53.1 (4)
C17—C18—C19—C20	0.6 (9)	C30—C29—P3—Rh2	125.1 (4)
C18—C19—C20—C15	0.4 (9)	C42—C41—P3—C35	−67.0 (3)
C16—C15—C20—C19	−0.5 (8)	C42—C41—P3—C29	−175.7 (3)
P2—C15—C20—C19	178.6 (4)	C42—C41—P3—Rh2	61.3 (3)
C26—C21—C22—C23	−1.1 (6)	C56—C55—P4—C49	175.6 (3)
P2—C21—C22—C23	−176.7 (3)	C56—C55—P4—C43	67.8 (4)
C21—C22—C23—C24	0.1 (7)	C56—C55—P4—Rh2	−61.0 (4)
C22—C23—C24—C25	1.4 (7)	C54—C49—P4—C55	0.0 (5)
C23—C24—C25—C26	−1.8 (8)	C50—C49—P4—C55	178.2 (4)
C24—C25—C26—C21	0.8 (8)	C54—C49—P4—C43	106.3 (4)
C22—C21—C26—C25	0.7 (7)	C50—C49—P4—C43	−75.5 (4)
P2—C21—C26—C25	176.3 (4)	C54—C49—P4—Rh2	−127.3 (4)
C34—C29—C30—C31	1.9 (7)	C50—C49—P4—Rh2	50.9 (4)
P3—C29—C30—C31	−176.3 (4)	C44—C43—P4—C55	−102.2 (4)
C29—C30—C31—C32	−3.0 (8)	C48—C43—P4—C55	74.3 (4)
C30—C31—C32—C33	2.3 (9)	C44—C43—P4—C49	149.8 (4)
C31—C32—C33—C34	−0.5 (8)	C48—C43—P4—C49	−33.8 (4)
C30—C29—C34—C33	−0.1 (7)	C44—C43—P4—Rh2	27.0 (4)
P3—C29—C34—C33	178.2 (4)	C48—C43—P4—Rh2	−156.6 (3)
C32—C33—C34—C29	−0.6 (8)	C13—P1—Rh1—C57B	27.4 (8)
C40—C35—C36—C37	0.2 (7)	C7—P1—Rh1—C57B	−91.9 (8)

P3—C35—C36—C37	−176.7 (3)	C1—P1—Rh1—C57B	148.0 (8)
C35—C36—C37—C38	−0.1 (7)	C13—P1—Rh1—C57	−154.3 (4)
C36—C37—C38—C39	−0.5 (8)	C7—P1—Rh1—C57	86.4 (4)
C37—C38—C39—C40	1.1 (7)	C1—P1—Rh1—C57	−33.7 (4)
C36—C35—C40—C39	0.4 (6)	C13—P1—Rh1—Cl1	24.7 (2)
P3—C35—C40—C39	177.2 (3)	C7—P1—Rh1—Cl1	−94.6 (2)
C38—C39—C40—C35	−1.0 (7)	C1—P1—Rh1—Cl1	145.30 (19)
C48—C43—C44—C45	0.5 (7)	C13—P1—Rh1—Cl1B	−156.3 (3)
P4—C43—C44—C45	177.0 (4)	C7—P1—Rh1—Cl1B	84.4 (3)
C43—C44—C45—C46	0.3 (8)	C1—P1—Rh1—Cl1B	−35.7 (3)
C44—C45—C46—C47	−0.3 (8)	C21—P2—Rh1—C57B	33.7 (8)
C45—C46—C47—C48	−0.6 (7)	C15—P2—Rh1—C57B	−86.2 (8)
C46—C47—C48—C43	1.5 (7)	C27—P2—Rh1—C57B	154.0 (8)
C44—C43—C48—C47	−1.4 (6)	C21—P2—Rh1—C57	−144.7 (4)
P4—C43—C48—C47	−177.9 (3)	C15—P2—Rh1—C57	95.5 (4)
C54—C49—C50—C51	−1.3 (8)	C27—P2—Rh1—C57	−24.3 (4)
P4—C49—C50—C51	−179.5 (4)	C21—P2—Rh1—Cl1	36.3 (2)
C49—C50—C51—C52	2.2 (8)	C15—P2—Rh1—Cl1	−83.5 (2)
C50—C51—C52—C53	−1.2 (9)	C27—P2—Rh1—Cl1	156.7 (2)
C51—C52—C53—C54	−0.7 (9)	C21—P2—Rh1—Cl1B	−142.7 (3)
C50—C49—C54—C53	−0.7 (7)	C15—P2—Rh1—Cl1B	97.5 (3)
P4—C49—C54—C53	177.5 (4)	C27—P2—Rh1—Cl1B	−22.3 (3)
C52—C53—C54—C49	1.7 (8)	C43—P4—Rh2—C58B	−144.0 (4)
C14—C13—P1—C7	−177.9 (3)	C55—P4—Rh2—C58	156.3 (5)
C14—C13—P1—C1	−69.1 (4)	C49—P4—Rh2—C58	−84.0 (5)
C14—C13—P1—Rh1	58.6 (4)	C43—P4—Rh2—C58	35.0 (5)
C8—C7—P1—C13	−160.7 (4)	C55—P4—Rh2—Cl2B	158.8 (2)
C12—C7—P1—C13	20.0 (5)	C49—P4—Rh2—Cl2B	−81.4 (2)
C8—C7—P1—C1	92.4 (4)	C43—P4—Rh2—Cl2B	37.5 (2)
C12—C7—P1—C1	−86.8 (4)	C55—P4—Rh2—Cl2	−20.8 (2)
C8—C7—P1—Rh1	−34.1 (5)	C49—P4—Rh2—Cl2	99.0 (2)
C12—C7—P1—Rh1	146.7 (4)	C43—P4—Rh2—Cl2	−142.1 (2)
C2—C1—P1—C13	−83.1 (4)	C35—P3—Rh2—C58B	−37.8 (4)
C6—C1—P1—C13	93.1 (4)	C29—P3—Rh2—C58B	81.2 (4)
C2—C1—P1—C7	24.9 (4)	C41—P3—Rh2—C58B	−159.5 (4)
C6—C1—P1—C7	−158.9 (4)	C35—P3—Rh2—C58	143.2 (5)
C2—C1—P1—Rh1	148.8 (3)	C29—P3—Rh2—C58	−97.8 (5)
C6—C1—P1—Rh1	−35.0 (4)	C41—P3—Rh2—C58	21.5 (5)
C22—C21—P2—C15	−28.8 (4)	C35—P3—Rh2—Cl2B	140.6 (2)
C26—C21—P2—C15	155.6 (4)	C29—P3—Rh2—Cl2B	−100.3 (2)
C22—C21—P2—C27	79.5 (4)	C41—P3—Rh2—Cl2B	19.0 (2)
C26—C21—P2—C27	−96.1 (4)	C35—P3—Rh2—Cl2	−39.8 (2)
C22—C21—P2—Rh1	−152.3 (3)	C29—P3—Rh2—Cl2	79.2 (2)
C26—C21—P2—Rh1	32.1 (4)	C41—P3—Rh2—Cl2	−161.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22—H22···O2^{i}	0.95	2.64	3.424 (18)	140
C48—H48···O1*B*^{ii}	0.95	2.68	3.51 (3)	145
C4—H4···O1*B*^{iii}	0.95	2.71	3.51 (3)	142

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+2; (ii) −*x*+2, *y*+1/2, −*z*+2; (iii) −*x*+2, *y*−1/2, −*z*+2.