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# *trans*-Carbonylchloridobis(ethyldiphenylphosphine-$\kappa P$)rhodium(I)

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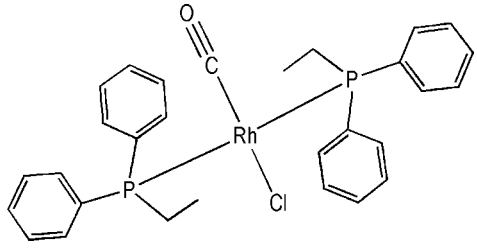
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.007 Å; disorder in main residue; $R$ factor = 0.037; $wR$ factor = 0.080; data-to-parameter ratio = 19.0.

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
$\beta$ = 90.216 (6)°
$V$ = 2645.3 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 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···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) $-x+1, y-\frac{1}{2}, -z+2$; (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).

## References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Beck, C. M., Rathmill, S. E., Park, Y. J., Chen, J., Crabtree, R. H., Liable-Sands, L. M. & Rheingold, A. L. (1999). *Organometallics*, **18**, 5311–5317 and references therein.
Bruker (1997). *SAINT*. Version 7.03A. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Higham, L. J., Whittlesey, M. K. & Wood, P. T. (2004). *J. Chem. Soc. Dalton Trans.* pp. 4202–4208.

 doi:10.1107/S1600536807065877  

Hoye, P. A. T., Pringle, P. G., Smith, M. B. & Worboys, K. (1993). *J. Chem. Soc. Dalton Trans.* pp. 269–274.
Lorenzini, F., Patrick, B. O. & James, B. R. (2007*a*). *J. Chem. Soc. Dalton Trans.* pp. 3224–3226.
Lorenzini, F., Patrick, B. O. & James, B. R. (2007*b*). *Inorg. Chem.* **46**, 8998–9002.
Lorenzini, F., Patrick, B. O. & James, B. R. (2007*c*). *Inorg. Chim. Acta*. doi: 10.1016/j.ica.2007.10.044. In the press.
O'Connor, C. & Wilkinson, G. (1969). *Tetrahedron Lett.* pp. 1375–1377.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Vallarino, L. (1957). *J. Chem. Soc.* pp. 2287–2292.
Vaska, L. & Di Luzio, J. W. (1961). *J. Am. Chem. Soc.* **83**, 2784–2785.
Vaska, L. & Di Luzio, J. W. (1962). *J. Am. Chem. Soc.* **84**, 679–680.

# supplementary materials

*Acta Cryst.* (2008). E**64**, m179-m180 [ **doi:10.1107/S1600536807065877** ]

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

**F. Lorenzini, B. O. Patrick and B. R. James**

## 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-phosphine)$_2$, where (P-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).

## 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 μ*L*, 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($PEtPh_2$)$_3$.

### 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.

### Figures

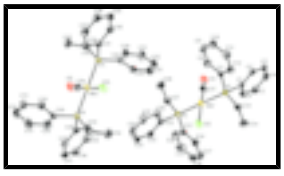

Fig. 1.

### *trans*-Carbonylchloridobis(ethyldiphenylphosphine-κ*P*)rhodium(I)

*Crystal data*

| | |
|---|---|
| [RhCl($C_{14}H_{15}P$)$_2$(CO)] | $F_{000}$ = 1216 |
| $M_r$ = 594.83 | $D_x$ = 1.494 Mg m$^{-3}$ |
| Monoclinic, $P2_1$ | Mo *K*α radiation<br>λ = 0.71073 Å |
| *a* = 9.8557 (14) Å | Cell parameters from 6687 reflections |
| *b* = 16.385 (2) Å | θ = 2.4–27.8º |
| *c* = 16.381 (2) Å | μ = 0.89 mm$^{-1}$ |
| β = 90.216 (6)º | *T* = 173.0 (1) K |
| *V* = 2645.3 (6) Å$^3$ | Prism, yellow |
| *Z* = 4 | 0.15 × 0.15 × 0.07 mm |

*Data collection*

| | |
|---|---|
| Bruker X8 APEXII diffractometer | 8610 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.049 |
| *T* = 173.0(1) K | $\theta_{max}$ = 28.0º |
| area–detector scans | $\theta_{min}$ = 1.8º |
| Absorption correction: multi-scan (SADABS; Bruker, 2003) | *h* = −12→12 |
| $T_{min}$ = 0.701, $T_{max}$ = 0.940 | *k* = −21→21 |
| 41680 measured reflections | *l* = −21→21 |

12665 independent reflections

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.037$ | $w = 1/[\sigma^2(F_o^2) + (0.0297P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.080$ | $(\Delta/\sigma)_{max} = 0.001$ |
| $S = 0.98$ | $\Delta\rho_{max} = 0.45$ e Å$^{-3}$ |
| 12665 reflections | $\Delta\rho_{min} = -0.36$ e Å$^{-3}$ |
| 668 parameters | Extinction correction: none |
| 1 restraint | Absolute structure: Flack (1983), 6047 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.04 (4) |
| Secondary atom site location: difference Fourier map | |

*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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, °)*

| | | | |
|---|---|---|---|
| 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) |

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| 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) |

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|---|---|---|---|
| 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) |

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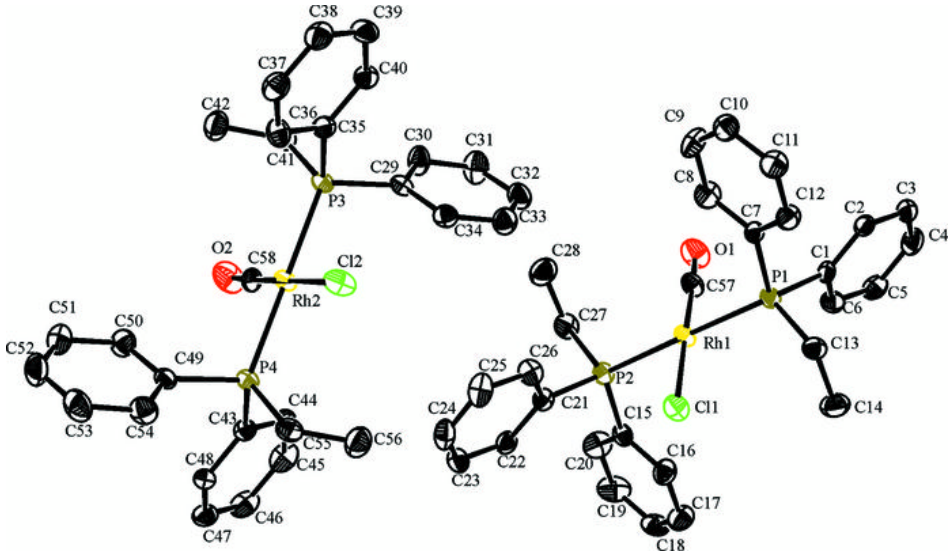
| P3—C35—C40—C39 | 177.2 (3) | C7—P1—Rh1—Cl1 | −94.6 (2) |
| C38—C39—C40—C35 | −1.0 (7) | C1—P1—Rh1—Cl1 | 145.30 (19) |
| C48—C43—C44—C45 | 0.5 (7) | C13—P1—Rh1—Cl1B | −156.3 (3) |
| P4—C43—C44—C45 | 177.0 (4) | C7—P1—Rh1—Cl1B | 84.4 (3) |
| C43—C44—C45—C46 | 0.3 (8) | C1—P1—Rh1—Cl1B | −35.7 (3) |
| 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, °)*

| *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*−1/2, −*z*+2; (ii) −*x*+2, *y*+1/2, −*z*+2; (iii) −*x*+2, *y*−1/2, −*z*+2.

**Fig. 1**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