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## Structure Reports

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# {Bis[2-(diphenylphosphino)ethyl]phenylphosphine- $\kappa^3 P, P', P''$ ]chlorido-palladium(II) hexafluoridophosphate

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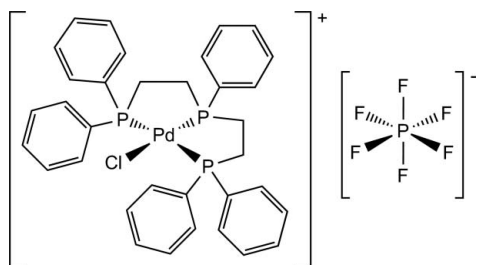
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.067; data-to-parameter ratio = 32.1.

In the title compound,  $[\text{PdCl}(\text{C}_{34}\text{H}_{33}\text{P}_3)]\text{PF}_6$ , the  $\text{Pd}^{\text{II}}$  atom adopts a distorted  $\text{PdP}_3\text{Cl}$  square-planar geometry arising from the  $P, P', P''$ -tridentate triphos ligand and a chloride ion.

## Related literature

For the synthesis, see: King *et al.* (1971). The corresponding complex with a  $\text{Pt}^{\text{II}}$  metal center is concurrently published (Heston *et al.*, 2009). The corresponding  $\text{Pd}^{\text{II}}$  complex has been previously reported as a trifluoromethanesulfonate salt (Müller *et al.*, 2000). The corresponding complexes with both  $\text{Pt}^{\text{II}}$  and  $\text{Pd}^{\text{II}}$  have been previously reported as chloride and diphenyltetrachloridostannate(IV) salts (Sevillano *et al.*, 1999a; Garcia-Seijo *et al.*, 2001; Housecroft *et al.*, 1990). For other group 10–triphos complexes, see: Sevillano *et al.* (1999b); Fernandez *et al.* (2005); Aizawa *et al.* (2002); Bertinsson *et al.* (1983); Autissier *et al.* (2005); Fernandez *et al.* (2005).



## Experimental

### Crystal data

 $[\text{PdCl}(\text{C}_{34}\text{H}_{33}\text{P}_3)]\text{PF}_6$   
 $M_r = 821.33$ 

 Triclinic,  $P\bar{1}$   
 $a = 11.2465$  (5) Å

 $b = 11.8182$  (5) Å  
 $c = 15.5093$  (7) Å  
 $\alpha = 69.029$  (2)°  
 $\beta = 70.439$  (2)°  
 $\gamma = 69.697$  (2)°  
 $V = 1752.27$  (13) Å<sup>3</sup>
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.84$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.47 \times 0.15 \times 0.10$  mm

### Data collection

 Bruker APEXII CCD  
 diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2000)  
 $T_{\text{min}} = 0.693$ ,  $T_{\text{max}} = 0.917$ 

 48576 measured reflections  
 13341 independent reflections  
 10917 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.030$ 

### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.067$   
 $S = 1.03$   
 13341 reflections

 415 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.71$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.67$  e Å<sup>-3</sup>
**Table 1**

Selected bond lengths (Å).

Pd1—P1	2.2176 (4)	Pd1—P3	2.3329 (4)
Pd1—P2	2.3178 (4)	Pd1—Cl1	2.3441 (4)

Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2006); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2992).

## References

- Aizawa, S., Sone, Y., Kawamoto, T., Yamada, S. & Nakamura, M. (2002). *Inorg. Chim. Acta*, **338**, 235–239.
- Autissier, V., Brockman, E., Clegg, W., Harrington, R. W. & Henderson, R. A. (2005). *J. Organomet. Chem.* **690**, 1763–1771.
- Bertinsson, G.-I. (1983). *Acta Cryst.* **C39**, 563–567.
- Bruker (2000). SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2006). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
- Fernandez, D., Garcia-Seijo, M. I., Sevillano, P., Castineiras, A. & Garcia-Fernandez, M. E. (2005). *Inorg. Chim. Acta*, **358**, 2575–2584.
- Garcia-Seijo, M. I., Castineiras, A., Mahieu, B., Janosi, L., Berente, Z., Kollar, L. & Garcia-Fernandez, M. E. (2001). *Polyhedron*, **20**, 855–868.
- Heston, S. A., Noll, B. C. & Helm, M. L. (2009). *Acta Cryst.* **E65**, m793.
- Housecroft, C. E., Shaykh, B. A. M., Rheingold, A. L. & Haggerty, B. S. (1990). *Acta Cryst.* **C46**, 1549–1551.
- King, R. B., Kapoor, P. N. & Kapoor, R. N. (1971). *Inorg. Chem.* **10**, 1841–1850.
- Müller, T. E., Grosche, M., Herdtweck, E., Pleier, A.-K., Walter, E. & Yaw-Kai, Y. (2000). *Organometallics*, **19**, 170–183.
- Sevillano, P., Habtemariam, A., Parsons, S., Castineiras, A., Garcia, M. E. & Sadler, P. J. (1999a). *J. Chem. Soc. Dalton Trans.* pp. 2861–2870.
- Sevillano, P., Habtemariam, A., Parsons, S., Castineiras, A., Garcia, M. E. & Sadler, P. J. (1999b). *Polyhedron*, **18**, 383–389.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.

## supporting information

*Acta Cryst.* (2009). E65, m792 [doi:10.1107/S1600536809022417]

**{Bis[2-(diphenylphosphino)ethyl]phenylphosphine- $\kappa^3P,P',P''$ ]chloridopalladium(II) hexafluoridophosphate**

**Paul R. Vorce, Susie M. Miller and Monte L. Helm**

**S1. Comment**

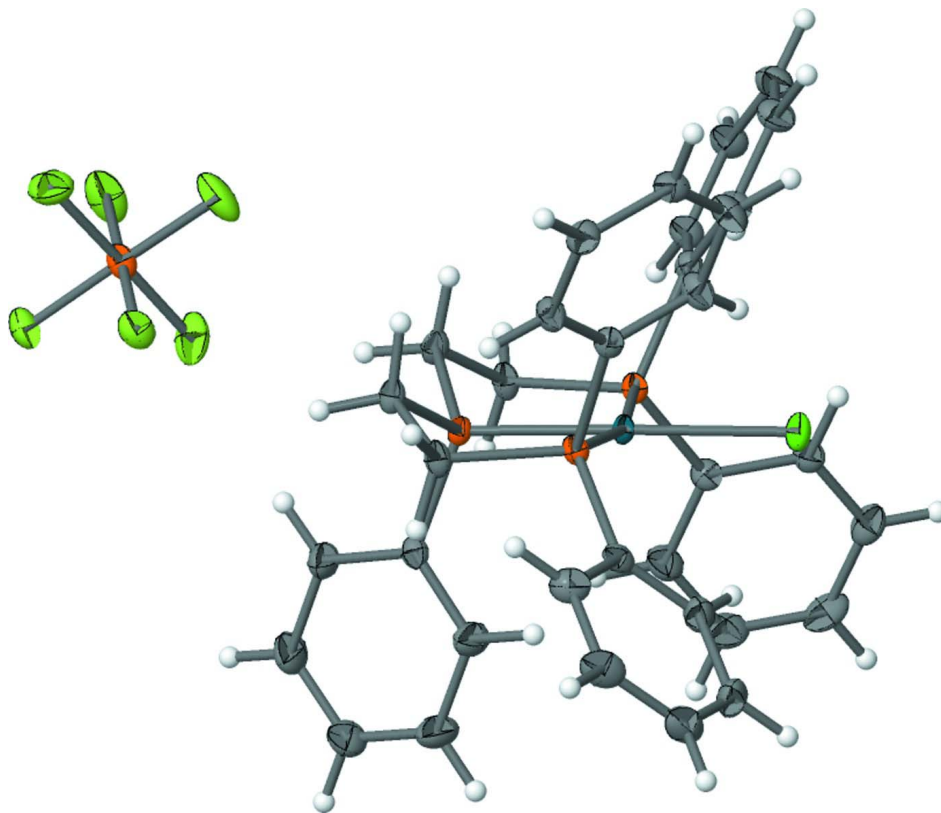
The crystal structure of the title compound, (I), consists of a  $[Pd(\text{triphos})Cl]^+$  cation and  $PF_6^-$  anion (Fig. 1). The cation shows a distorted square planar geometry around the metal center and the charge is balanced by a non-coordinating  $PF_6^-$  anion.

**S2. Experimental**

The title compound was prepared by a previously reported procedure (King, *et al.*, 1971). Colourless rods of (I) were grown by slow solvent evaporation of a saturated dichloromethane solution.

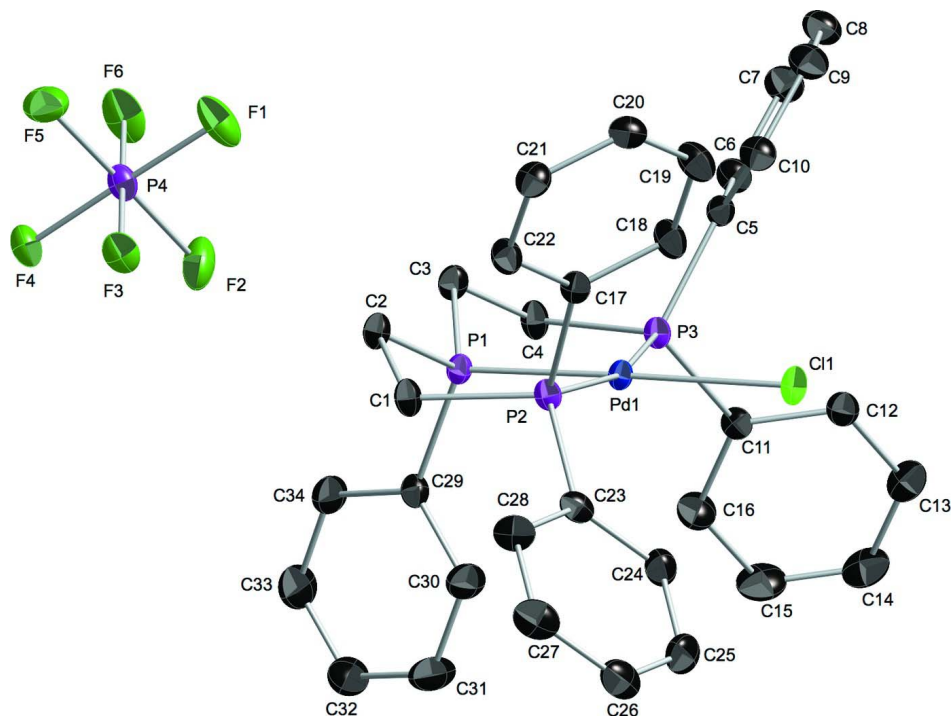
**S3. Refinement**

All H atoms were placed in calculated positions ( $C-H = 0.93-0.97\text{\AA}$ ) and refined as riding with  $U_{iso}(H) = 1.2U_{eq}(C)$ .



**Figure 1**

The molecular structure of (I) with 50% probability displacement ellipsoids.



**Figure 2**

The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids. Hydrogen atoms are omitted for clarity.

**{Bis[2-(diphenylphosphino)ethyl]phenylphosphine- $\kappa^3P,P',P''$ }chloridopalladium(II) hexafluoridophosphate**

*Crystal data*

[PdCl(C<sub>34</sub>H<sub>33</sub>P<sub>3</sub>)]PF<sub>6</sub>

$M_r = 821.33$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 11.2465 (5) \text{ \AA}$

$b = 11.8182 (5) \text{ \AA}$

$c = 15.5093 (7) \text{ \AA}$

$\alpha = 69.029 (2)^\circ$

$\beta = 70.439 (2)^\circ$

$\gamma = 69.697 (2)^\circ$

$V = 1752.27 (13) \text{ \AA}^3$

$Z = 2$

$F(000) = 828$

$D_x = 1.557 \text{ Mg m}^{-3}$

Melting point: not measured K

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 9890 reflections

$\theta = 2.7\text{--}33.3^\circ$

$\mu = 0.84 \text{ mm}^{-1}$

$T = 100 \text{ K}$

Rod, colourless

$0.47 \times 0.15 \times 0.10 \text{ mm}$

*Data collection*

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2000)

$T_{\min} = 0.693$ ,  $T_{\max} = 0.917$

48576 measured reflections

13341 independent reflections

10917 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 33.4^\circ$ ,  $\theta_{\min} = 1.9^\circ$

$h = -16 \rightarrow 17$

$k = -18 \rightarrow 18$

$l = -23 \rightarrow 21$

Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.067$   
 $S = 1.03$   
 13341 reflections  
 415 parameters  
 0 restraints  
 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0249P)^2 + 0.7353P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.002$   
 $\Delta\rho_{\max} = 0.71 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.67 \text{ e } \text{\AA}^{-3}$

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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Pd1	0.543690 (10)	0.544468 (10)	0.728992 (7)	0.01221 (3)
Cl1	0.66556 (3)	0.69224 (3)	0.64082 (3)	0.01911 (7)
P1	0.41725 (3)	0.41349 (3)	0.80705 (3)	0.01332 (7)
P2	0.34703 (3)	0.69724 (3)	0.73350 (3)	0.01374 (7)
P3	0.71382 (3)	0.36524 (3)	0.75901 (3)	0.01384 (7)
C1	0.63963 (14)	0.23211 (14)	0.82230 (11)	0.0178 (3)
H1A	0.6334	0.1964	0.7756	0.021*
H1B	0.6956	0.1658	0.8631	0.021*
C2	0.50294 (14)	0.27458 (14)	0.88395 (11)	0.0177 (3)
H2A	0.5089	0.2948	0.9388	0.021*
H2B	0.4566	0.2077	0.9082	0.021*
C3	0.26481 (14)	0.49798 (14)	0.87132 (11)	0.0182 (3)
H3A	0.2009	0.4465	0.9003	0.022*
H3B	0.2800	0.5191	0.9224	0.022*
C4	0.21432 (13)	0.61759 (14)	0.79763 (11)	0.0184 (3)
H4A	0.1379	0.6736	0.8297	0.022*
H4B	0.1869	0.5962	0.7523	0.022*
C5	0.32177 (14)	0.80673 (14)	0.79914 (10)	0.0156 (3)
C6	0.19906 (14)	0.89177 (15)	0.81373 (11)	0.0197 (3)
H6A	0.1315	0.8893	0.7911	0.024*
C7	0.17601 (16)	0.97952 (16)	0.86117 (12)	0.0242 (3)
H7A	0.0925	1.0370	0.8713	0.029*
C8	0.27491 (17)	0.98361 (16)	0.89391 (12)	0.0261 (4)
H8A	0.2591	1.0444	0.9260	0.031*
C9	0.39634 (16)	0.89942 (17)	0.87998 (12)	0.0250 (3)

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H9A	0.4634	0.9022	0.9029	0.030*
C10	0.42046 (15)	0.81067 (15)	0.83243 (11)	0.0207 (3)
H10A	0.5039	0.7531	0.8228	0.025*
C11	0.31785 (13)	0.79486 (14)	0.61900 (10)	0.0158 (3)
C12	0.35593 (15)	0.90719 (15)	0.57975 (11)	0.0193 (3)
H12A	0.3897	0.9338	0.6156	0.023*
C13	0.34469 (16)	0.97972 (16)	0.48887 (12)	0.0259 (4)
H13A	0.3710	1.0557	0.4625	0.031*
C14	0.29516 (17)	0.94151 (18)	0.43648 (12)	0.0305 (4)
H14A	0.2872	0.9913	0.3742	0.037*
C15	0.25735 (19)	0.8311 (2)	0.47485 (13)	0.0337 (4)
H15A	0.2228	0.8055	0.4389	0.040*
C16	0.26919 (17)	0.75693 (18)	0.56544 (13)	0.0271 (4)
H16A	0.2441	0.6803	0.5909	0.033*
C17	0.79995 (13)	0.37155 (14)	0.83702 (10)	0.0156 (3)
C18	0.81699 (16)	0.48626 (15)	0.82975 (12)	0.0222 (3)
H18A	0.7779	0.5608	0.7880	0.027*
C19	0.89105 (16)	0.49210 (16)	0.88346 (13)	0.0245 (3)
H19A	0.9026	0.5705	0.8781	0.029*
C20	0.94768 (14)	0.38410 (15)	0.94455 (11)	0.0200 (3)
H20A	0.9981	0.3883	0.9812	0.024*
C21	0.93115 (15)	0.26977 (16)	0.95254 (11)	0.0211 (3)
H21A	0.9708	0.1956	0.9943	0.025*
C22	0.85680 (15)	0.26298 (15)	0.89975 (11)	0.0201 (3)
H22A	0.8446	0.1845	0.9062	0.024*
C23	0.84173 (13)	0.31713 (15)	0.66107 (11)	0.0173 (3)
C24	0.85893 (17)	0.40133 (16)	0.57143 (12)	0.0253 (3)
H24A	0.8039	0.4843	0.5612	0.030*
C25	0.95762 (18)	0.36365 (18)	0.49618 (13)	0.0327 (4)
H25A	0.9700	0.4211	0.4347	0.039*
C26	1.03721 (16)	0.24272 (18)	0.51127 (14)	0.0304 (4)
H26A	1.1042	0.2173	0.4600	0.037*
C27	1.01997 (16)	0.15849 (18)	0.60052 (13)	0.0286 (4)
H27A	1.0747	0.0754	0.6102	0.034*
C28	0.92312 (15)	0.19491 (16)	0.67579 (12)	0.0231 (3)
H28A	0.9119	0.1372	0.7372	0.028*
C29	0.37076 (14)	0.36381 (14)	0.72824 (11)	0.0170 (3)
C30	0.43949 (16)	0.37635 (18)	0.63357 (12)	0.0264 (4)
H30A	0.5137	0.4095	0.6100	0.032*
C31	0.40025 (19)	0.3407 (2)	0.57341 (13)	0.0337 (4)
H31A	0.4483	0.3484	0.5091	0.040*
C32	0.29116 (19)	0.29404 (19)	0.60692 (13)	0.0313 (4)
H32A	0.2642	0.2702	0.5655	0.038*
C33	0.2214 (2)	0.2821 (2)	0.70068 (14)	0.0359 (5)
H33A	0.1459	0.2511	0.7233	0.043*
C34	0.26129 (17)	0.31525 (18)	0.76138 (12)	0.0289 (4)
H34A	0.2142	0.3050	0.8260	0.035*
P4	0.21871 (4)	0.13320 (4)	1.11479 (3)	0.01765 (8)

F1	0.14268 (9)	0.04474 (9)	1.10733 (7)	0.0233 (2)
F2	0.23404 (11)	0.04420 (10)	1.21717 (7)	0.0334 (2)
F3	0.35426 (8)	0.05090 (9)	1.06650 (7)	0.0241 (2)
F4	0.29314 (10)	0.22256 (10)	1.12031 (9)	0.0334 (3)
F5	0.20332 (10)	0.22185 (10)	1.01037 (8)	0.0341 (3)
F6	0.08134 (9)	0.21610 (10)	1.16043 (9)	0.0359 (3)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pd1	0.01063 (5)	0.00951 (5)	0.01375 (5)	-0.00185 (3)	-0.00232 (3)	-0.00135 (4)
Cl1	0.01759 (15)	0.01486 (17)	0.02136 (17)	-0.00688 (13)	-0.00301 (13)	0.00013 (13)
P1	0.01253 (15)	0.01079 (17)	0.01399 (16)	-0.00290 (13)	-0.00164 (12)	-0.00189 (13)
P2	0.01197 (15)	0.01054 (17)	0.01684 (17)	-0.00140 (12)	-0.00385 (13)	-0.00272 (13)
P3	0.01189 (15)	0.01076 (17)	0.01771 (17)	-0.00135 (13)	-0.00379 (13)	-0.00387 (14)
C1	0.0156 (6)	0.0118 (7)	0.0239 (7)	-0.0031 (5)	-0.0050 (5)	-0.0026 (6)
C2	0.0174 (6)	0.0135 (7)	0.0188 (7)	-0.0043 (5)	-0.0045 (5)	-0.0001 (5)
C3	0.0151 (6)	0.0159 (7)	0.0193 (7)	-0.0039 (5)	0.0005 (5)	-0.0044 (6)
C4	0.0133 (6)	0.0129 (7)	0.0255 (7)	-0.0031 (5)	-0.0019 (5)	-0.0041 (6)
C5	0.0170 (6)	0.0122 (7)	0.0156 (6)	-0.0024 (5)	-0.0044 (5)	-0.0025 (5)
C6	0.0180 (6)	0.0178 (7)	0.0232 (7)	-0.0020 (6)	-0.0060 (6)	-0.0072 (6)
C7	0.0242 (7)	0.0193 (8)	0.0272 (8)	-0.0009 (6)	-0.0040 (6)	-0.0107 (7)
C8	0.0322 (8)	0.0220 (8)	0.0270 (8)	-0.0052 (7)	-0.0079 (7)	-0.0112 (7)
C9	0.0268 (8)	0.0274 (9)	0.0263 (8)	-0.0076 (7)	-0.0105 (6)	-0.0092 (7)
C10	0.0198 (7)	0.0208 (8)	0.0218 (7)	-0.0023 (6)	-0.0081 (6)	-0.0059 (6)
C11	0.0137 (6)	0.0138 (7)	0.0189 (7)	-0.0003 (5)	-0.0066 (5)	-0.0040 (5)
C12	0.0211 (7)	0.0158 (7)	0.0201 (7)	-0.0033 (6)	-0.0065 (6)	-0.0038 (6)
C13	0.0264 (8)	0.0199 (8)	0.0229 (8)	-0.0027 (6)	-0.0062 (6)	0.0010 (6)
C14	0.0279 (8)	0.0363 (10)	0.0194 (8)	-0.0009 (7)	-0.0116 (7)	-0.0002 (7)
C15	0.0347 (9)	0.0471 (12)	0.0274 (9)	-0.0119 (9)	-0.0166 (8)	-0.0099 (9)
C16	0.0310 (8)	0.0294 (9)	0.0278 (9)	-0.0122 (7)	-0.0122 (7)	-0.0067 (7)
C17	0.0130 (6)	0.0133 (7)	0.0179 (7)	-0.0010 (5)	-0.0030 (5)	-0.0043 (5)
C18	0.0245 (7)	0.0138 (7)	0.0293 (8)	-0.0023 (6)	-0.0129 (6)	-0.0037 (6)
C19	0.0258 (8)	0.0186 (8)	0.0347 (9)	-0.0047 (6)	-0.0128 (7)	-0.0094 (7)
C20	0.0162 (6)	0.0237 (8)	0.0213 (7)	-0.0029 (6)	-0.0053 (5)	-0.0091 (6)
C21	0.0212 (7)	0.0205 (8)	0.0199 (7)	-0.0038 (6)	-0.0082 (6)	-0.0022 (6)
C22	0.0227 (7)	0.0145 (7)	0.0229 (7)	-0.0045 (6)	-0.0080 (6)	-0.0029 (6)
C23	0.0136 (6)	0.0197 (7)	0.0224 (7)	-0.0052 (5)	-0.0033 (5)	-0.0100 (6)
C24	0.0296 (8)	0.0197 (8)	0.0252 (8)	-0.0102 (7)	0.0011 (6)	-0.0080 (7)
C25	0.0392 (10)	0.0307 (10)	0.0258 (9)	-0.0207 (8)	0.0096 (7)	-0.0098 (8)
C26	0.0206 (7)	0.0380 (11)	0.0365 (10)	-0.0127 (7)	0.0074 (7)	-0.0228 (8)
C27	0.0181 (7)	0.0313 (10)	0.0370 (10)	0.0007 (7)	-0.0048 (7)	-0.0188 (8)
C28	0.0186 (7)	0.0244 (8)	0.0251 (8)	0.0008 (6)	-0.0076 (6)	-0.0093 (7)
C29	0.0179 (6)	0.0135 (7)	0.0188 (7)	-0.0043 (5)	-0.0056 (5)	-0.0022 (5)
C30	0.0228 (7)	0.0368 (10)	0.0224 (8)	-0.0134 (7)	-0.0001 (6)	-0.0107 (7)
C31	0.0355 (9)	0.0511 (13)	0.0214 (8)	-0.0196 (9)	-0.0027 (7)	-0.0136 (8)
C32	0.0380 (10)	0.0370 (11)	0.0283 (9)	-0.0175 (8)	-0.0132 (7)	-0.0071 (8)
C33	0.0402 (10)	0.0468 (12)	0.0322 (10)	-0.0302 (9)	-0.0076 (8)	-0.0065 (9)

C34	0.0325 (9)	0.0381 (11)	0.0220 (8)	-0.0231 (8)	-0.0022 (7)	-0.0055 (7)
P4	0.01521 (16)	0.01243 (18)	0.0248 (2)	-0.00147 (14)	-0.00703 (14)	-0.00449 (15)
F1	0.0217 (4)	0.0182 (5)	0.0329 (5)	-0.0076 (4)	-0.0095 (4)	-0.0054 (4)
F2	0.0469 (6)	0.0305 (6)	0.0226 (5)	-0.0058 (5)	-0.0139 (5)	-0.0061 (4)
F3	0.0169 (4)	0.0213 (5)	0.0338 (5)	-0.0021 (4)	-0.0041 (4)	-0.0118 (4)
F4	0.0237 (5)	0.0232 (5)	0.0630 (8)	-0.0036 (4)	-0.0147 (5)	-0.0214 (5)
F5	0.0362 (6)	0.0240 (5)	0.0363 (6)	-0.0103 (5)	-0.0185 (5)	0.0098 (5)
F6	0.0185 (4)	0.0226 (5)	0.0633 (8)	0.0007 (4)	-0.0014 (5)	-0.0216 (5)

*Geometric parameters (Å, °)*

Pd1—P1	2.2176 (4)	C15—C16	1.387 (3)
Pd1—P2	2.3178 (4)	C15—H15A	0.9500
Pd1—P3	2.3329 (4)	C16—H16A	0.9500
Pd1—C11	2.3441 (4)	C17—C18	1.394 (2)
P1—C29	1.8073 (16)	C17—C22	1.398 (2)
P1—C3	1.8193 (14)	C18—C19	1.392 (2)
P1—C2	1.8211 (15)	C18—H18A	0.9500
P2—C11	1.8037 (15)	C19—C20	1.381 (2)
P2—C5	1.8126 (15)	C19—H19A	0.9500
P2—C4	1.8476 (15)	C20—C21	1.384 (2)
P3—C23	1.8132 (15)	C20—H20A	0.9500
P3—C17	1.8185 (16)	C21—C22	1.389 (2)
P3—C1	1.8418 (15)	C21—H21A	0.9500
C1—C2	1.534 (2)	C22—H22A	0.9500
C1—H1A	0.9900	C23—C24	1.387 (2)
C1—H1B	0.9900	C23—C28	1.401 (2)
C2—H2A	0.9900	C24—C25	1.398 (2)
C2—H2B	0.9900	C24—H24A	0.9500
C3—C4	1.532 (2)	C25—C26	1.383 (3)
C3—H3A	0.9900	C25—H25A	0.9500
C3—H3B	0.9900	C26—C27	1.383 (3)
C4—H4A	0.9900	C26—H26A	0.9500
C4—H4B	0.9900	C27—C28	1.385 (2)
C5—C10	1.392 (2)	C27—H27A	0.9500
C5—C6	1.399 (2)	C28—H28A	0.9500
C6—C7	1.384 (2)	C29—C30	1.393 (2)
C6—H6A	0.9500	C29—C34	1.402 (2)
C7—C8	1.389 (2)	C30—C31	1.388 (3)
C7—H7A	0.9500	C30—H30A	0.9500
C8—C9	1.384 (2)	C31—C32	1.385 (3)
C8—H8A	0.9500	C31—H31A	0.9500
C9—C10	1.393 (2)	C32—C33	1.384 (3)
C9—H9A	0.9500	C32—H32A	0.9500
C10—H10A	0.9500	C33—C34	1.382 (3)
C11—C16	1.390 (2)	C33—H33A	0.9500
C11—C12	1.399 (2)	C34—H34A	0.9500
C12—C13	1.384 (2)	P4—F1	1.6158 (10)



C12—H12A	0.9500	P4—F2	1.5872 (11)
C13—C14	1.384 (3)	P4—F3	1.5997 (10)
C13—H13A	0.9500	P4—F4	1.5967 (11)
C14—C15	1.378 (3)	P4—F6	1.6005 (10)
C14—H14A	0.9500	P4—F5	1.6117 (11)
P1—Pd1—P2	83.905 (14)	C14—C15—H15A	120.1
P1—Pd1—P3	84.262 (14)	C16—C15—H15A	120.1
P2—Pd1—P3	166.221 (13)	C15—C16—C11	119.90 (17)
P1—Pd1—C11	175.897 (14)	C15—C16—H16A	120.1
P2—Pd1—C11	92.644 (14)	C11—C16—H16A	120.1
P3—Pd1—C11	99.430 (14)	C18—C17—C22	119.14 (15)
C29—P1—C3	105.15 (7)	C18—C17—P3	119.17 (12)
C29—P1—C2	108.28 (7)	C22—C17—P3	121.56 (12)
C3—P1—C2	113.38 (7)	C19—C18—C17	120.29 (15)
C29—P1—Pd1	112.53 (5)	C19—C18—H18A	120.1
C3—P1—Pd1	107.87 (5)	C17—C18—H18A	120.1
C2—P1—Pd1	109.64 (5)	C20—C19—C18	120.05 (15)
C11—P2—C5	104.67 (7)	C20—C19—H19A	120.1
C11—P2—C4	108.65 (7)	C18—C19—H19A	120.1
C5—P2—C4	104.60 (7)	C19—C20—C21	120.16 (15)
C11—P2—Pd1	115.24 (5)	C19—C20—H20A	120.1
C5—P2—Pd1	115.29 (5)	C21—C20—H20A	120.1
C4—P2—Pd1	107.76 (5)	C20—C21—C22	120.26 (15)
C23—P3—C17	104.71 (7)	C20—C21—H21A	120.1
C23—P3—C1	105.01 (7)	C22—C21—H21A	120.1
C17—P3—C1	106.71 (7)	C21—C22—C17	120.09 (15)
C23—P3—Pd1	120.12 (5)	C21—C22—H22A	120.1
C17—P3—Pd1	112.42 (5)	C17—C22—H22A	120.1
C1—P3—Pd1	106.97 (5)	C24—C23—C28	119.94 (14)
C1—C2—H2A	109.7	C24—C23—P3	119.98 (12)
P1—C2—H2A	111.0	C28—C23—P3	120.07 (12)
C1—C2—H2B	109.7	C23—C24—C25	119.72 (16)
P1—C2—H2B	111.0	C23—C24—H24A	120.1
C2—C1—P3	110.54 (10)	C25—C24—H24A	120.1
C2—C1—H1A	109.7	C26—C25—C24	119.95 (17)
P3—C1—H1A	109.7	C26—C25—H25A	120.1
C2—C1—H1B	109.7	C24—C25—H25A	120.1
P3—C1—H1B	109.7	C25—C26—C27	120.43 (15)
C1—C2—P1	106.09 (10)	C25—C26—H26A	120.1
C4—C3—P1	106.05 (10)	C27—C26—H26A	120.1
C4—C3—H3A	109.7	C26—C27—C28	120.18 (17)
P1—C3—H3A	111.0	C26—C27—H27A	120.1
C4—C3—H3B	109.7	C28—C27—H27A	120.1
P1—C3—H3B	111.0	C27—C28—C23	119.77 (16)
C3—C4—P2	108.46 (10)	C27—C28—H28A	120.1
C3—C4—H4A	109.7	C23—C28—H28A	120.1
P2—C4—H4A	111.0	C30—C29—C34	118.84 (15)

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C3—C4—H4B	109.7	C30—C29—P1	121.20 (12)
P3—C4—H4B	103.0	C34—C29—P1	119.94 (12)
C10—C5—C6	119.82 (14)	C31—C30—C29	120.39 (15)
C10—C5—P2	122.34 (11)	C31—C30—H30A	120.1
C6—C5—P2	117.82 (12)	C29—C30—H30A	120.1
C7—C6—C5	120.02 (15)	C32—C31—C30	120.12 (16)
C7—C6—H6A	120.1	C32—C31—H31A	120.1
C5—C6—H6A	120.1	C30—C31—H31A	120.1
C6—C7—C8	120.02 (15)	C33—C32—C31	120.01 (17)
C6—C7—H7A	120.1	C33—C32—H32A	120.1
C8—C7—H7A	120.1	C31—C32—H32A	120.1
C9—C8—C7	120.21 (16)	C34—C33—C32	120.17 (16)
C9—C8—H8A	120.1	C34—C33—H33A	120.1
C7—C8—H8A	120.1	C32—C33—H33A	120.1
C8—C9—C10	120.21 (16)	C33—C34—C29	120.46 (16)
C8—C9—H9A	120.1	C33—C34—H34A	120.1
C10—C9—H9A	120.1	C29—C34—H34A	120.1
C5—C10—C9	119.72 (15)	F2—P4—F4	91.25 (6)
C5—C10—H10A	120.1	F2—P4—F3	90.49 (6)
C9—C10—H10A	120.1	F4—P4—F3	90.41 (5)
C16—C11—C12	119.14 (14)	F2—P4—F6	90.92 (6)
C16—C11—P2	121.99 (12)	F4—P4—F6	90.63 (6)
C12—C11—P2	118.63 (12)	F3—P4—F6	178.24 (6)
C13—C12—C11	120.33 (15)	F2—P4—F5	179.18 (6)
C13—C12—H12A	120.1	F4—P4—F5	89.44 (6)
C11—C12—H12A	120.1	F3—P4—F5	89.06 (6)
C14—C13—C12	120.02 (16)	F6—P4—F5	89.53 (6)
C14—C13—H13A	120.1	F2—P4—F1	89.86 (6)
C12—C13—H13A	120.1	F4—P4—F1	178.88 (6)
C15—C14—C13	119.87 (16)	F3—P4—F1	89.74 (5)
C15—C14—H14A	120.1	F6—P4—F1	89.19 (5)
C13—C14—H14A	120.1	F5—P4—F1	89.45 (6)
C14—C15—C16	120.72 (17)		

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