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# Di-$\mu$-diphenylphosphido-bis{chlorido-[(mesitylmethyl)diphenylphosphine-$\kappa P$]-palladium(II)}

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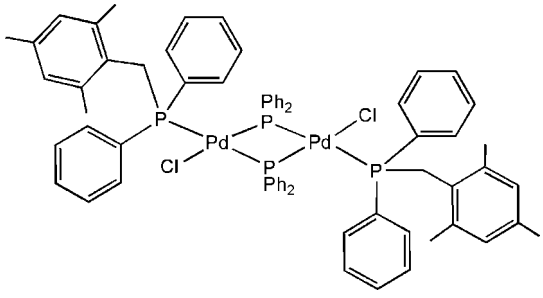
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.031; $wR$ factor = 0.064; data-to-parameter ratio = 17.4.

In the title dinuclear palladium complex, $[Pd_2(C_{12}H_{10}P)_2Cl_2(C_{22}H_{23}P)_2]$, the terminal ligands adopt a trans configuration with a Pd···Pd distance of 3.6111 (4) Å. A crystallographic twofold rotation axis runs perpendicular to the $Pd_2P_2$ ring. The Cl atom lies slightly out of the plane of the Pd and three P atoms in each half of the molecule.

## Related literature

For similar dinuclear palladium complexes, see: Brandon & Dixon (1981); Carty *et al.* (1982); Gebauer *et al.* (1992); Zhuravel *et al.* (2000). For the synthesis of $PPh_2CH_2(2,4,6\text{-}Me_3C_6H_2)$, see: Chahen *et al.* (2006).




## Experimental

### Crystal data

$[Pd_2(C_{12}H_{10}P)_2Cl_2(C_{22}H_{23}P)_2]$
$M_r$ = 1290.83
Orthorhombic, *Pccn*
$a$ = 12.0793 (7) Å
$b$ = 22.6156 (14) Å
$c$ = 22.5499 (14) Å
$V$ = 6160.2 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.81 mm$^{-1}$
$T$ = 173 (2) K
0.31 × 0.24 × 0.17 mm

### Data collection

Stoe IPDS diffractometer
Absorption correction: none
46413 measured reflections
6011 independent reflections
3498 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.089

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.064
$S$ = 0.78
6011 reflections
346 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.98 e Å$^{-3}$

Data collection: *EXPOSE* in *IPDS Software* (Stoe & Cie, 2000); cell refinement: *CELL* in *IPDS Software*; data reduction: *INTEGRATE* in *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Version 1.4.1; Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2205).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m1989 [ **doi:10.1107/S1600536807030280** ]

# Di-$\mu$-diphenylphosphido-bis{chlorido[(mesitylmethyl)diphenylphosphine-$\kappa P$]palladium(II)}

**L. Chahen, B. Therrien and G. Süss-Fink**

## Comment

The title compound, $[PdCl(\mu_2\text{-}PPh_2)\{PPh_2CH_2(2,4,6\text{-}Me_3C_6H_2)\}]_2$, (I), is prepared in a similar manner as the isoelectronic dinuclear palladium complex $[PdCl(\mu_2\text{-}PPh_2)(PPh_3)]_2$ (Brandon & Dixon, 1981). The triphenylphosphine being replaced by (mesithylmethyl)(diphenyl)phosphine (Chahen *et al.*, 2006). The $^{31}P\{^1H\}$ NMR spectrum gives rise to two multiplets centred at 7.5 and −142.6 p.p.m. respectively. The signals are consistent with an AA'BB' spin system (Brandon & Dixon, 1981). The molecular structure of (I) shows the palladium atoms to be surrounded by two phosphido-bridged ligands, a chloride, and a $PPh_2CH_2(2,4,6\text{-}Me_3C_6H_2)$ ligand. The complex adopts the *trans*-symmetrical isomer, see scheme.

The two halves of the dinuclear complex are related by a crystallography twofold rotation axis, see Fig. 1. The Pd atoms are in a slightly distorted square-planar geometry. The plane formed by the palladium, the chloride and the three P atoms is mainly planar, with a maximum deviation from the mean plane of 0.0770 (4)Å for one bridging P atom. However, the angle between the two square-planar units is 12.63 (1)°, giving rise to a slightly bent conformation for the dimeric unit, see Fig. 2. Otherwise, the bond distances and angles are similar to those found in $[PtCl(\mu_2\text{-}PPh_2)(HPPh_2)]_2$ (Carty *et al.*, 1982), $[PdCl(\mu_2\text{-}PPh_2)(HPPh_2)]_2$ (Gebauer *et al.*, 1992) and $[PdI(\mu_2\text{-}PPh_2)(HPPh_2)]_2$ (Zhuravel *et al.*, 2000).

## Experimental

The synthesis of $[PdCl(\mu_2\text{-}PPh_2)\{PPh_2CH_2(2,4,6\text{-}Me_3C_6H_2)\}]_2$ is identical to the synthesis of $[PdCl(\mu_2\text{-}PPh_2)(PPh_3)]_2$ (Brandon & Dixon, 1981). The yellow product is purified by column chromatography on silica gel (dichloromethane:acetone, 1:2).

$^1H$ NMR ($CDCl_3$): 6.9–6.2 (m, 44H), 2.76 (m, 4H), 1.58 (s, 12H), 1.34 (m, 6H). $^{31}P$ NMR ($CDCl_3$): 7.5 and −142.6 p.p.m.. MS (ESI, m/*z*): 1291; $[C_{68}H_{66}Cl_2P_4Pd_2]$ Calcd. for $C_{68}H_{66}Cl_2P_4Pd_2$: C, 63.27; H, 5.15 Found: C, 62.87; H, 5.02.

$[PdCl(\mu_2\text{-}PPh_2)\{PPh_2CH_2(2,4,6\text{-}Me_3C_6H_2)\}]_2$ is disolved in chloroform, and crystals suitable for X-ray diffraction analysis are obtained by slow evaporation of the chloroform solution.

## Refinement

The H atoms were included in calculated positions and refined using a riding model, with C—H = 0.93–0.96 Å and with $U_{iso}(H)$ = 1.2 (1.5 for methyl groups) times $U_{eq}(C)$.

## Figures

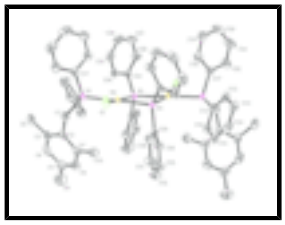

Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

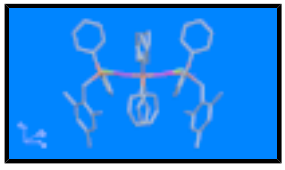

Fig. 2. Bent conformation adopted by the title compound.

## Di-μ-diphenylphosphido-bis{chlorido[(mesitylmethyl)diphenylphosphine- κ*P*]palladium(II)]}

### *Crystal data*

| | |
|---|---|
| $[Pd_2(C_{12}H_{10}P)_2Cl_2(C_{22}H_{23}P)_2]$ | $F_{000}$ = 2640 |
| $M_r$ = 1290.83 | $D_x$ = 1.392 Mg m$^{-3}$ |
| Orthorhombic, *Pccn* | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ab 2ac | Cell parameters from 8000 reflections |
| *a* = 12.0793 (7) Å | θ = 2.1–25.9º |
| *b* = 22.6156 (14) Å | μ = 0.81 mm$^{-1}$ |
| *c* = 22.5499 (14) Å | *T* = 173 (2) K |
| *V* = 6160.2 (6) Å$^3$ | Plate, yellow |
| *Z* = 4 | 0.31 × 0.24 × 0.17 mm |

### *Data collection*

| | |
|---|---|
| Stoe IPDS<br>diffractometer | 6011 independent reflections |
| Radiation source: fine-focus sealed tube | 3498 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.089 |
| Detector resolution: 0.81 pixels mm$^{-1}$ | $\theta_{max}$ = 26.0º |
| *T* = 173(2) K | $\theta_{min}$ = 2.0º |
| φ oscillation scans | *h* = −14→14 |
| Absorption correction: none | *k* = −27→27 |
| 46413 measured reflections | *l* = −27→27 |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.031 | H-atom parameters constrained |

| | |
|---|---|
| $wR(F^2) = 0.064$ | $w = 1/[\sigma^2(F_o^2) + (0.0284P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 0.78$ | $(\Delta/\sigma)_{max} = 0.002$ |
| 6011 reflections | $\Delta\rho_{max} = 0.53$ e Å$^{-3}$ |
| 346 parameters | $\Delta\rho_{min} = -0.98$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Special details*

**Experimental**. A crystal was mounted at 173 K on a Stoe Image Plate Diffraction System (Stoe, 2000) using Mo *K*α graphite monochromated radiation. Image plate distance 70 mm, φ oscillation scans 0 − 200°, step Δφ = 1.0°, 3 minutes per frame.

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.3394 (2) | 0.68728 (15) | 0.14638 (15) | 0.0288 (8) |
| H1A | 0.3333 | 0.7299 | 0.1498 | 0.035* |
| H1B | 0.2726 | 0.6729 | 0.1273 | 0.035* |
| C2 | 0.3467 (2) | 0.66113 (15) | 0.20757 (16) | 0.0313 (8) |
| C3 | 0.2996 (3) | 0.60533 (16) | 0.21955 (18) | 0.0348 (9) |
| C4 | 0.3181 (3) | 0.57908 (17) | 0.27389 (19) | 0.0446 (10) |
| H4 | 0.2867 | 0.5423 | 0.2813 | 0.054* |
| C5 | 0.3810 (3) | 0.60503 (18) | 0.31752 (19) | 0.0467 (10) |
| C6 | 0.4210 (3) | 0.66176 (18) | 0.30728 (18) | 0.0442 (10) |
| H6 | 0.4601 | 0.6810 | 0.3371 | 0.053* |
| C7 | 0.4040 (3) | 0.69051 (15) | 0.25328 (16) | 0.0332 (8) |
| C8 | 0.2300 (3) | 0.57336 (17) | 0.17367 (18) | 0.0455 (10) |
| H8A | 0.2078 | 0.5356 | 0.1890 | 0.068* |
| H8B | 0.2726 | 0.5678 | 0.1382 | 0.068* |
| H8C | 0.1654 | 0.5965 | 0.1648 | 0.068* |
| C9 | 0.4049 (4) | 0.5717 (2) | 0.3747 (2) | 0.0758 (14) |
| H9A | 0.3390 | 0.5517 | 0.3876 | 0.114* |
| H9B | 0.4282 | 0.5991 | 0.4047 | 0.114* |
| H9C | 0.4625 | 0.5433 | 0.3679 | 0.114* |
| C10 | 0.4471 (3) | 0.75305 (17) | 0.24475 (16) | 0.0434 (9) |
| H10A | 0.3857 | 0.7799 | 0.2420 | 0.065* |
| H10B | 0.4899 | 0.7550 | 0.2090 | 0.065* |
| H10C | 0.4927 | 0.7638 | 0.2779 | 0.065* |

| | | | | |
|---|---|---|---|---|
| C11 | 0.4922 (2) | 0.59215 (13) | 0.11434 (15) | 0.0257 (8) |
| C12 | 0.4717 (3) | 0.54607 (15) | 0.07458 (17) | 0.0335 (9) |
| H12 | 0.4377 | 0.5538 | 0.0384 | 0.040* |
| C13 | 0.5023 (3) | 0.48856 (15) | 0.08905 (17) | 0.0379 (10) |
| H13 | 0.4872 | 0.4579 | 0.0628 | 0.045* |
| C14 | 0.5544 (3) | 0.47669 (17) | 0.14176 (19) | 0.0409 (10) |
| H14 | 0.5772 | 0.4384 | 0.1504 | 0.049* |
| C15 | 0.5733 (3) | 0.52168 (16) | 0.18205 (18) | 0.0364 (9) |
| H15 | 0.6068 | 0.5135 | 0.2183 | 0.044* |
| C16 | 0.5420 (2) | 0.57898 (15) | 0.16824 (17) | 0.0304 (8) |
| H16 | 0.5545 | 0.6091 | 0.1955 | 0.036* |
| C17 | 0.4122 (2) | 0.67027 (14) | 0.02220 (15) | 0.0279 (8) |
| C18 | 0.4917 (3) | 0.67252 (16) | −0.02190 (16) | 0.0372 (9) |
| H18 | 0.5662 | 0.6716 | −0.0117 | 0.045* |
| C19 | 0.4618 (3) | 0.67611 (17) | −0.08118 (17) | 0.0443 (10) |
| H19 | 0.5163 | 0.6770 | −0.1103 | 0.053* |
| C20 | 0.3531 (3) | 0.67830 (17) | −0.09702 (19) | 0.0508 (11) |
| H20 | 0.3329 | 0.6810 | −0.1367 | 0.061* |
| C21 | 0.2743 (3) | 0.6765 (2) | −0.0539 (2) | 0.0614 (13) |
| H21 | 0.2000 | 0.6780 | −0.0646 | 0.074* |
| C22 | 0.3022 (3) | 0.67225 (18) | 0.00542 (18) | 0.0475 (11) |
| H22 | 0.2469 | 0.6708 | 0.0341 | 0.057* |
| C23 | 0.7748 (2) | 0.63475 (14) | 0.04978 (15) | 0.0256 (8) |
| C24 | 0.7492 (3) | 0.57485 (15) | 0.05565 (16) | 0.0324 (8) |
| H24 | 0.7251 | 0.5605 | 0.0921 | 0.039* |
| C25 | 0.7593 (3) | 0.53672 (18) | 0.00822 (18) | 0.0466 (10) |
| H25 | 0.7424 | 0.4969 | 0.0130 | 0.056* |
| C26 | 0.7940 (3) | 0.5572 (2) | −0.0457 (2) | 0.0540 (12) |
| H26 | 0.8001 | 0.5314 | −0.0777 | 0.065* |
| C27 | 0.8196 (3) | 0.6159 (2) | −0.05260 (18) | 0.0527 (11) |
| H27 | 0.8432 | 0.6297 | −0.0894 | 0.063* |
| C28 | 0.8109 (3) | 0.65508 (17) | −0.00562 (16) | 0.0378 (9) |
| H28 | 0.8289 | 0.6947 | −0.0108 | 0.045* |
| C29 | 0.7848 (2) | 0.65141 (14) | 0.17945 (16) | 0.0262 (8) |
| C30 | 0.8636 (3) | 0.60701 (15) | 0.18551 (18) | 0.0357 (9) |
| H30 | 0.9022 | 0.5934 | 0.1526 | 0.043* |
| C31 | 0.8840 (3) | 0.58332 (18) | 0.2410 (2) | 0.0500 (11) |
| H31 | 0.9355 | 0.5530 | 0.2450 | 0.060* |
| C32 | 0.8293 (3) | 0.6039 (2) | 0.2902 (2) | 0.0550 (12) |
| H32 | 0.8440 | 0.5875 | 0.3272 | 0.066* |
| C33 | 0.7531 (4) | 0.64862 (19) | 0.28494 (17) | 0.0513 (11) |
| H33 | 0.7170 | 0.6631 | 0.3183 | 0.062* |
| C34 | 0.7303 (3) | 0.67193 (16) | 0.22955 (16) | 0.0375 (9) |
| H34 | 0.6778 | 0.7018 | 0.2258 | 0.045* |
| Cl1 | 0.46039 (6) | 0.81271 (4) | 0.08771 (4) | 0.0368 (2) |
| P3 | 0.76040 (6) | 0.68822 (3) | 0.10901 (4) | 0.02197 (18) |
| P5 | 0.46032 (6) | 0.66918 (4) | 0.09866 (4) | 0.02419 (19) |
| Pd1 | 0.601393 (16) | 0.741408 (10) | 0.103340 (11) | 0.02204 (7) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0208 (15) | 0.033 (2) | 0.033 (2) | 0.0008 (14) | 0.0053 (14) | −0.0005 (17) |
| C2 | 0.0270 (17) | 0.035 (2) | 0.032 (2) | 0.0045 (15) | 0.0070 (15) | 0.0018 (18) |
| C3 | 0.0304 (17) | 0.038 (2) | 0.037 (2) | 0.0009 (16) | 0.0071 (16) | −0.0002 (19) |
| C4 | 0.039 (2) | 0.042 (2) | 0.052 (3) | −0.0029 (18) | 0.012 (2) | 0.010 (2) |
| C5 | 0.048 (2) | 0.055 (3) | 0.037 (3) | 0.002 (2) | 0.006 (2) | 0.007 (2) |
| C6 | 0.045 (2) | 0.055 (3) | 0.033 (3) | 0.0003 (19) | 0.0029 (18) | −0.004 (2) |
| C7 | 0.0287 (16) | 0.036 (2) | 0.034 (2) | 0.0011 (17) | 0.0073 (17) | −0.0054 (17) |
| C8 | 0.042 (2) | 0.046 (3) | 0.048 (3) | −0.0153 (18) | 0.0046 (18) | 0.005 (2) |
| C9 | 0.095 (4) | 0.081 (4) | 0.052 (3) | −0.002 (3) | −0.010 (3) | 0.024 (3) |
| C10 | 0.0496 (19) | 0.045 (2) | 0.036 (2) | −0.0038 (19) | 0.0057 (16) | −0.010 (2) |
| C11 | 0.0238 (15) | 0.0244 (17) | 0.029 (2) | 0.0010 (13) | 0.0014 (14) | 0.0013 (16) |
| C12 | 0.0353 (18) | 0.033 (2) | 0.033 (2) | −0.0068 (15) | −0.0013 (16) | 0.0033 (17) |
| C13 | 0.048 (2) | 0.0225 (19) | 0.043 (3) | −0.0054 (16) | 0.0112 (18) | −0.0054 (18) |
| C14 | 0.046 (2) | 0.029 (2) | 0.048 (3) | 0.0036 (16) | 0.0113 (19) | 0.007 (2) |
| C15 | 0.0339 (19) | 0.038 (2) | 0.038 (3) | 0.0032 (15) | 0.0048 (16) | 0.0130 (19) |
| C16 | 0.0228 (16) | 0.032 (2) | 0.037 (2) | 0.0005 (14) | 0.0033 (15) | 0.0003 (18) |
| C17 | 0.0299 (17) | 0.0249 (18) | 0.029 (2) | −0.0019 (15) | −0.0042 (15) | −0.0012 (15) |
| C18 | 0.0399 (19) | 0.040 (2) | 0.031 (2) | −0.0046 (17) | 0.0001 (17) | 0.0013 (19) |
| C19 | 0.062 (3) | 0.042 (2) | 0.029 (2) | −0.0030 (19) | 0.0041 (19) | −0.0003 (19) |
| C20 | 0.070 (3) | 0.053 (2) | 0.029 (3) | 0.0086 (19) | −0.016 (2) | 0.000 (2) |
| C21 | 0.046 (3) | 0.090 (4) | 0.048 (3) | 0.011 (2) | −0.024 (2) | −0.006 (3) |
| C22 | 0.0335 (19) | 0.070 (3) | 0.039 (3) | 0.0002 (19) | −0.0039 (18) | −0.001 (2) |
| C23 | 0.0205 (17) | 0.030 (2) | 0.026 (2) | 0.0043 (13) | −0.0024 (13) | −0.0059 (16) |
| C24 | 0.0297 (15) | 0.032 (2) | 0.036 (2) | −0.0042 (15) | 0.0036 (19) | −0.0080 (18) |
| C25 | 0.046 (2) | 0.042 (2) | 0.052 (3) | −0.0046 (18) | 0.001 (2) | −0.019 (2) |
| C26 | 0.059 (2) | 0.061 (3) | 0.042 (3) | 0.002 (2) | −0.002 (2) | −0.028 (2) |
| C27 | 0.063 (3) | 0.076 (3) | 0.019 (2) | 0.007 (2) | 0.002 (2) | −0.005 (2) |
| C28 | 0.047 (2) | 0.041 (2) | 0.026 (2) | 0.0048 (17) | −0.0022 (18) | −0.0015 (19) |
| C29 | 0.0283 (17) | 0.0248 (19) | 0.026 (2) | −0.0061 (14) | −0.0016 (14) | 0.0050 (16) |
| C30 | 0.0361 (19) | 0.036 (2) | 0.035 (2) | 0.0031 (15) | −0.0041 (16) | 0.0025 (18) |
| C31 | 0.055 (2) | 0.043 (2) | 0.052 (3) | 0.010 (2) | −0.018 (2) | 0.014 (2) |
| C32 | 0.064 (3) | 0.068 (3) | 0.032 (3) | −0.006 (2) | −0.013 (2) | 0.019 (2) |
| C33 | 0.059 (2) | 0.070 (3) | 0.025 (2) | −0.003 (2) | 0.005 (2) | 0.007 (2) |
| C34 | 0.041 (2) | 0.039 (2) | 0.032 (2) | 0.0016 (16) | −0.0012 (16) | 0.0034 (19) |
| Cl1 | 0.0234 (4) | 0.0269 (5) | 0.0601 (7) | 0.0045 (3) | −0.0014 (4) | 0.0051 (4) |
| P3 | 0.0207 (4) | 0.0218 (4) | 0.0234 (5) | 0.0006 (3) | 0.0003 (4) | 0.0009 (4) |
| P5 | 0.0200 (4) | 0.0234 (4) | 0.0291 (5) | −0.0016 (3) | 0.0004 (4) | 0.0007 (4) |
| Pd1 | 0.01932 (10) | 0.02174 (12) | 0.02506 (13) | 0.00082 (11) | −0.00015 (11) | 0.00017 (13) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.504 (5) | C18—C19 | 1.387 (5) |
| C1—P5 | 1.860 (3) | C18—H18 | 0.9300 |
| C1—H1A | 0.9700 | C19—C20 | 1.362 (5) |
| C1—H1B | 0.9700 | C19—H19 | 0.9300 |

| | | | |
|---|---|---|---|
| C2—C7 | 1.408 (5) | C20—C21 | 1.361 (6) |
| C2—C3 | 1.410 (5) | C20—H20 | 0.9300 |
| C3—C4 | 1.380 (5) | C21—C22 | 1.382 (6) |
| C3—C8 | 1.517 (5) | C21—H21 | 0.9300 |
| C4—C5 | 1.375 (5) | C22—H22 | 0.9300 |
| C4—H4 | 0.9300 | C23—C24 | 1.396 (4) |
| C5—C6 | 1.390 (5) | C23—C28 | 1.401 (5) |
| C5—C9 | 1.521 (6) | C23—P3 | 1.810 (3) |
| C6—C7 | 1.396 (5) | C24—C25 | 1.379 (5) |
| C6—H6 | 0.9300 | C24—H24 | 0.9300 |
| C7—C10 | 1.519 (5) | C25—C26 | 1.368 (6) |
| C8—H8A | 0.9600 | C25—H25 | 0.9300 |
| C8—H8B | 0.9600 | C26—C27 | 1.373 (6) |
| C8—H8C | 0.9600 | C26—H26 | 0.9300 |
| C9—H9A | 0.9600 | C27—C28 | 1.385 (5) |
| C9—H9B | 0.9600 | C27—H27 | 0.9300 |
| C9—H9C | 0.9600 | C28—H28 | 0.9300 |
| C10—H10A | 0.9600 | C29—C34 | 1.388 (5) |
| C10—H10B | 0.9600 | C29—C30 | 1.390 (4) |
| C10—H10C | 0.9600 | C29—P3 | 1.817 (3) |
| C11—C16 | 1.388 (5) | C30—C31 | 1.383 (5) |
| C11—C12 | 1.397 (5) | C30—H30 | 0.9300 |
| C11—P5 | 1.819 (3) | C31—C32 | 1.372 (6) |
| C12—C13 | 1.391 (5) | C31—H31 | 0.9300 |
| C12—H12 | 0.9300 | C32—C33 | 1.373 (6) |
| C13—C14 | 1.372 (5) | C32—H32 | 0.9300 |
| C13—H13 | 0.9300 | C33—C34 | 1.383 (5) |
| C14—C15 | 1.383 (5) | C33—H33 | 0.9300 |
| C14—H14 | 0.9300 | C34—H34 | 0.9300 |
| C15—C16 | 1.385 (5) | Cl1—Pd1 | 2.3718 (8) |
| C15—H15 | 0.9300 | P3—Pd1 | 2.2699 (8) |
| C16—H16 | 0.9300 | P3—Pd1$^{i}$ | 2.3101 (8) |
| C17—C18 | 1.383 (5) | P5—Pd1 | 2.3629 (8) |
| C17—C22 | 1.383 (4) | Pd1—P3$^{i}$ | 2.3101 (8) |
| C17—P5 | 1.819 (3) | | |
| C2—C1—P5 | 113.5 (2) | C20—C19—C18 | 120.4 (4) |
| C2—C1—H1A | 108.9 | C20—C19—H19 | 119.8 |
| P5—C1—H1A | 108.9 | C18—C19—H19 | 119.8 |
| C2—C1—H1B | 108.9 | C21—C20—C19 | 119.0 (4) |
| P5—C1—H1B | 108.9 | C21—C20—H20 | 120.5 |
| H1A—C1—H1B | 107.7 | C19—C20—H20 | 120.5 |
| C7—C2—C3 | 118.7 (3) | C20—C21—C22 | 121.5 (4) |
| C7—C2—C1 | 121.0 (3) | C20—C21—H21 | 119.2 |
| C3—C2—C1 | 120.3 (3) | C22—C21—H21 | 119.2 |
| C4—C3—C2 | 119.3 (4) | C21—C22—C17 | 120.1 (4) |
| C4—C3—C8 | 119.4 (3) | C21—C22—H22 | 120.0 |
| C2—C3—C8 | 121.3 (3) | C17—C22—H22 | 120.0 |
| C5—C4—C3 | 122.8 (4) | C24—C23—C28 | 118.2 (3) |

| | | | |
|---|---|---|---|
| C5—C4—H4 | 118.6 | C24—C23—P3 | 123.9 (3) |
| C3—C4—H4 | 118.6 | C28—C23—P3 | 117.9 (3) |
| C4—C5—C6 | 117.9 (4) | C25—C24—C23 | 120.9 (4) |
| C4—C5—C9 | 120.0 (4) | C25—C24—H24 | 119.5 |
| C6—C5—C9 | 122.1 (4) | C23—C24—H24 | 119.5 |
| C5—C6—C7 | 121.6 (4) | C26—C25—C24 | 120.3 (4) |
| C5—C6—H6 | 119.2 | C26—C25—H25 | 119.8 |
| C7—C6—H6 | 119.2 | C24—C25—H25 | 119.8 |
| C6—C7—C2 | 119.4 (3) | C25—C26—C27 | 119.8 (4) |
| C6—C7—C10 | 119.6 (3) | C25—C26—H26 | 120.1 |
| C2—C7—C10 | 121.0 (3) | C27—C26—H26 | 120.1 |
| C3—C8—H8A | 109.5 | C26—C27—C28 | 121.0 (4) |
| C3—C8—H8B | 109.5 | C26—C27—H27 | 119.5 |
| H8A—C8—H8B | 109.5 | C28—C27—H27 | 119.5 |
| C3—C8—H8C | 109.5 | C27—C28—C23 | 119.8 (4) |
| H8A—C8—H8C | 109.5 | C27—C28—H28 | 120.1 |
| H8B—C8—H8C | 109.5 | C23—C28—H28 | 120.1 |
| C5—C9—H9A | 109.5 | C34—C29—C30 | 119.1 (3) |
| C5—C9—H9B | 109.5 | C34—C29—P3 | 118.8 (3) |
| H9A—C9—H9B | 109.5 | C30—C29—P3 | 121.9 (3) |
| C5—C9—H9C | 109.5 | C31—C30—C29 | 119.4 (4) |
| H9A—C9—H9C | 109.5 | C31—C30—H30 | 120.3 |
| H9B—C9—H9C | 109.5 | C29—C30—H30 | 120.3 |
| C7—C10—H10A | 109.5 | C32—C31—C30 | 120.9 (4) |
| C7—C10—H10B | 109.5 | C32—C31—H31 | 119.5 |
| H10A—C10—H10B | 109.5 | C30—C31—H31 | 119.5 |
| C7—C10—H10C | 109.5 | C31—C32—C33 | 120.2 (4) |
| H10A—C10—H10C | 109.5 | C31—C32—H32 | 119.9 |
| H10B—C10—H10C | 109.5 | C33—C32—H32 | 119.9 |
| C16—C11—C12 | 118.6 (3) | C32—C33—C34 | 119.4 (4) |
| C16—C11—P5 | 117.9 (3) | C32—C33—H33 | 120.3 |
| C12—C11—P5 | 123.5 (3) | C34—C33—H33 | 120.3 |
| C13—C12—C11 | 120.0 (3) | C33—C34—C29 | 120.9 (4) |
| C13—C12—H12 | 120.0 | C33—C34—H34 | 119.5 |
| C11—C12—H12 | 120.0 | C29—C34—H34 | 119.5 |
| C14—C13—C12 | 120.5 (3) | C23—P3—C29 | 108.87 (16) |
| C14—C13—H13 | 119.7 | C23—P3—Pd1 | 113.18 (10) |
| C12—C13—H13 | 119.7 | C29—P3—Pd1 | 115.42 (11) |
| C13—C14—C15 | 120.1 (4) | C23—P3—Pd1$^{i}$ | 110.50 (10) |
| C13—C14—H14 | 120.0 | C29—P3—Pd1$^{i}$ | 104.28 (10) |
| C15—C14—H14 | 120.0 | Pd1—P3—Pd1$^{i}$ | 104.08 (3) |
| C14—C15—C16 | 119.7 (4) | C11—P5—C17 | 105.36 (15) |
| C14—C15—H15 | 120.2 | C11—P5—C1 | 105.35 (15) |
| C16—C15—H15 | 120.2 | C17—P5—C1 | 107.13 (15) |
| C15—C16—C11 | 121.1 (3) | C11—P5—Pd1 | 120.04 (10) |
| C15—C16—H16 | 119.5 | C17—P5—Pd1 | 105.25 (10) |
| C11—C16—H16 | 119.5 | C1—P5—Pd1 | 112.86 (11) |
| C18—C17—C22 | 118.0 (3) | P3—Pd1—P3$^{i}$ | 75.55 (3) |

| | | | |
|---|---|---|---|
| C18—C17—P5 | 117.4 (2) | P3—Pd1—P5 | 104.26 (3) |
| C22—C17—P5 | 124.5 (3) | P3$^{i}$—Pd1—P5 | 179.37 (4) |
| C17—C18—C19 | 121.0 (3) | P3—Pd1—Cl1 | 167.50 (3) |
| C17—C18—H18 | 119.5 | P3$^{i}$—Pd1—Cl1 | 93.37 (3) |
| C19—C18—H18 | 119.5 | P5—Pd1—Cl1 | 86.87 (3) |
| P5—C1—C2—C7 | 85.3 (3) | C31—C32—C33—C34 | 1.2 (6) |
| P5—C1—C2—C3 | −92.2 (3) | C32—C33—C34—C29 | −1.1 (6) |
| C7—C2—C3—C4 | −4.9 (5) | C30—C29—C34—C33 | −0.3 (5) |
| C1—C2—C3—C4 | 172.6 (3) | P3—C29—C34—C33 | −174.6 (3) |
| C7—C2—C3—C8 | 175.6 (3) | C24—C23—P3—C29 | 31.2 (3) |
| C1—C2—C3—C8 | −6.9 (5) | C28—C23—P3—C29 | −150.5 (2) |
| C2—C3—C4—C5 | 0.0 (5) | C24—C23—P3—Pd1 | −98.5 (3) |
| C8—C3—C4—C5 | 179.5 (3) | C28—C23—P3—Pd1 | 79.7 (2) |
| C3—C4—C5—C6 | 4.3 (6) | C24—C23—P3—Pd1$^{i}$ | 145.2 (2) |
| C3—C4—C5—C9 | −175.6 (4) | C28—C23—P3—Pd1$^{i}$ | −36.6 (3) |
| C4—C5—C6—C7 | −3.7 (6) | C34—C29—P3—C23 | −149.4 (3) |
| C9—C5—C6—C7 | 176.2 (4) | C30—C29—P3—C23 | 36.5 (3) |
| C5—C6—C7—C2 | −1.1 (5) | C34—C29—P3—Pd1 | −20.9 (3) |
| C5—C6—C7—C10 | 178.6 (3) | C30—C29—P3—Pd1 | 165.0 (2) |
| C3—C2—C7—C6 | 5.5 (5) | C34—C29—P3—Pd1$^{i}$ | 92.6 (3) |
| C1—C2—C7—C6 | −172.1 (3) | C30—C29—P3—Pd1$^{i}$ | −81.5 (3) |
| C3—C2—C7—C10 | −174.2 (3) | C16—C11—P5—C17 | 173.5 (2) |
| C1—C2—C7—C10 | 8.3 (5) | C12—C11—P5—C17 | −5.0 (3) |
| C16—C11—C12—C13 | −0.8 (5) | C16—C11—P5—C1 | −73.4 (3) |
| P5—C11—C12—C13 | 177.6 (2) | C12—C11—P5—C1 | 108.1 (3) |
| C11—C12—C13—C14 | −1.2 (5) | C16—C11—P5—Pd1 | 55.2 (3) |
| C12—C13—C14—C15 | 2.5 (5) | C12—C11—P5—Pd1 | −123.2 (2) |
| C13—C14—C15—C16 | −1.8 (5) | C18—C17—P5—C11 | −83.7 (3) |
| C14—C15—C16—C11 | −0.3 (5) | C22—C17—P5—C11 | 100.0 (3) |
| C12—C11—C16—C15 | 1.5 (4) | C18—C17—P5—C1 | 164.5 (3) |
| P5—C11—C16—C15 | −177.0 (2) | C22—C17—P5—C1 | −11.8 (3) |
| C22—C17—C18—C19 | −0.6 (5) | C18—C17—P5—Pd1 | 44.1 (3) |
| P5—C17—C18—C19 | −177.1 (3) | C22—C17—P5—Pd1 | −132.2 (3) |
| C17—C18—C19—C20 | 0.9 (6) | C2—C1—P5—C11 | 40.5 (3) |
| C18—C19—C20—C21 | −0.5 (6) | C2—C1—P5—C17 | 152.3 (2) |
| C19—C20—C21—C22 | −0.2 (7) | C2—C1—P5—Pd1 | −92.3 (2) |
| C20—C21—C22—C17 | 0.5 (7) | C23—P3—Pd1—P3$^{i}$ | −126.54 (12) |
| C18—C17—C22—C21 | −0.1 (6) | C29—P3—Pd1—P3$^{i}$ | 107.09 (11) |
| P5—C17—C22—C21 | 176.2 (3) | Pd1$^{i}$—P3—Pd1—P3$^{i}$ | −6.53 (5) |
| C28—C23—C24—C25 | 0.0 (5) | C23—P3—Pd1—P5 | 54.08 (13) |
| P3—C23—C24—C25 | 178.3 (3) | C29—P3—Pd1—P5 | −72.29 (12) |
| C23—C24—C25—C26 | −0.4 (6) | Pd1$^{i}$—P3—Pd1—P5 | 174.09 (3) |
| C24—C25—C26—C27 | 0.5 (6) | C23—P3—Pd1—Cl1 | −98.4 (2) |
| C25—C26—C27—C28 | −0.1 (6) | C29—P3—Pd1—Cl1 | 135.22 (18) |
| C26—C27—C28—C23 | −0.3 (6) | Pd1$^{i}$—P3—Pd1—Cl1 | 21.60 (18) |
| C24—C23—C28—C27 | 0.4 (5) | C11—P5—Pd1—P3 | 11.84 (14) |

| | | | |
|---|---|---|---|
| P3—C23—C28—C27 | −178.0 (3) | C17—P5—Pd1—P3 | −106.51 (11) |
| C34—C29—C30—C31 | 1.5 (5) | C1—P5—Pd1—P3 | 136.98 (12) |
| P3—C29—C30—C31 | 175.6 (3) | C11—P5—Pd1—Cl1 | −173.91 (14) |
| C29—C30—C31—C32 | −1.4 (6) | C17—P5—Pd1—Cl1 | 67.74 (11) |
| C30—C31—C32—C33 | 0.0 (6) | C1—P5—Pd1—Cl1 | −48.76 (12) |

Symmetry codes: (i) −*x*+3/2, −*y*+3/2, *z*.

**Fig. 1**

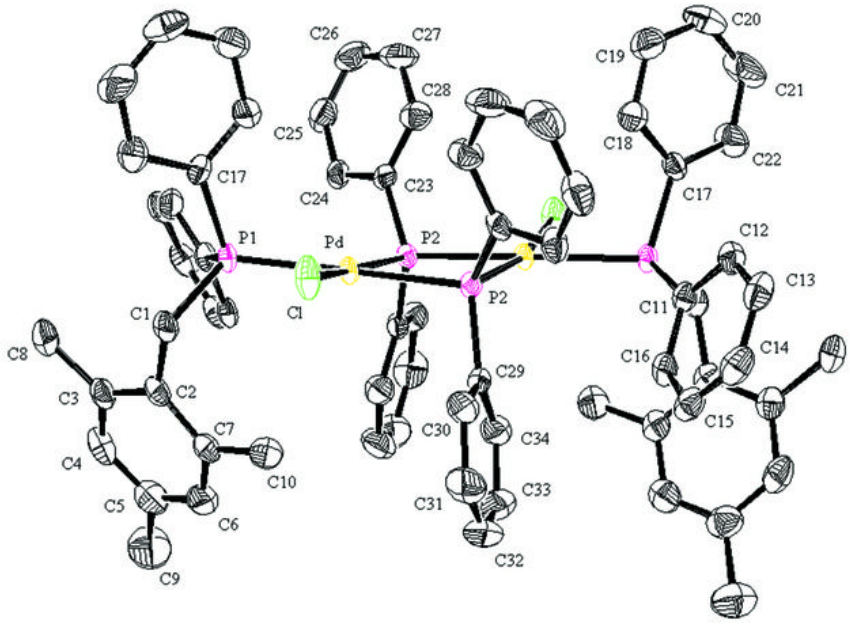
C26
C27
C28
C25
C24
C23
C17
P1
Pd
P2
Cl
C1
C8
C3
C2
C7
C4
C10
C5
C6
C9
C20
C19
C21
C18
C22
C17
C12
C13
C11
C16
C14
C15
P2
C29
C30
C34
C31
C33
C32

**Fig. 2**