Acta Crystallographica Section C
**Crystal Structure Communications**
ISSN 0108-2701

# Dichlorido{*N*-[2-(diphenylphosphanyl)benzylidene]-2-methylaniline}-palladium(II) acetonitrile monosolvate

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Received 21 January 2013
Accepted 23 January 2013
Online 5 February 2013

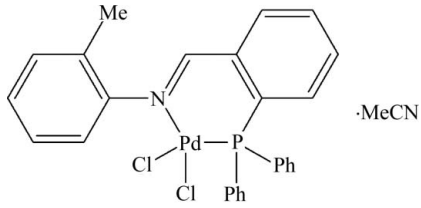
The title imino–phosphine compound, $[PdCl_2(C_{26}H_{22}NP)]\cdot CH_3CN$, was prepared by reaction of *N*-[2-(diphenylphosphanyl)benzylidene]-2-methylaniline with dichlorido(cyclooocta-1,5-diene)palladium(II) in dry $CH_2Cl_2$. The $Pd^{II}$ cation is coordinated by the P and N atoms of the bidentate chelating ligand and by two chloride anions, generating a distorted square-planar coordination geometry. There is a detectable *trans* influence for the chloride ligands. The methyl group present in this structure has an influence on the crystal packing.

## Comment

Imino–phosphine complexes have been studied since the early 1990s (Newkome, 1993; Ghilardi *et al.*, 1992). Their preparation is versatile because a wide range of amines and aldehydes of varying steric bulk are either available commercially or can be easily synthesized (Mogorosi *et al.*, 2011; Nobre & Monteiro, 2009; Pellagati *et al.*, 2005; Newkome, 1993; Ghilardi *et al.*, 1992; Vaughan *et al.*, 2011; Puri *et al.*, 2011; Doherty *et al.*, 2002; Onani *et al.*, 2010; Motswainyana *et al.*, 2012). The soft P atom coordinates strongly to soft metals, while the hard N atom is weakly coordinated and therefore more easily displaced, thus allowing hemilability. The hemilability of these ligands provides a unique reversible protection of coordination sites, an important property of ligands which leads to improved catalytic reactions (Ojwach *et al.*, 2007).

Phosphine-based complexes have been less well explored for their potential to inhibit tumour growth, possibly due to their susceptibility to oxidation, which makes them very difficult to handle in air. In our attempt to prepare new imino–phosphine palladium(II) complexes, which could induce apoptosis in tumour cells, we synthesized and crystallized the title compound, (I).

Compound (I) has proved to possess remarkable antiproliferative activities against the human breast (MCF-7) and human colon (HT-29) cancer cell lines compared with the reference drug cisplatin. The recorded cytotoxic activities could be attributed to the higher aqueous solubility of this palladium(II) complex, which makes it easier to dissociate in solution, thereby making the compound bio-available (Gao *et al.*, 2009). The imino–phosphine ligand *N*-[2-(diphenylphosphanyl)benzylidene]-2-methylaniline forms a six-membered ring around the metal centre, which stabilizes the complex during biological investigations, probably resulting in the observed antitumour profiles (Bacchi *et al.*, 2000).




(I)

The $Pd^{II}$ cation in (I) (Fig. 1) is coordinated by the P and N atoms of the imino–phosphine ligand and two chloride anions, generating a distorted square-planar coordination geometry around the metal centre. The bond angles around Pd1 (Table 1) describe the observed distorted square-planar geometry, while also indicating some ring strain induced by the chelating nature of the bidentate ligand. The Pd—C1 bond lengths (Table 1) are in good agreement with the average Pd—Cl bond length of 2.298 (15) Å for known palladium(II) complexes (Allen, 2002; Chiririwa & Muller, 2012). The average Pd—N and Pd—P bond lengths (Table 1) also compare well with literature values (Chiririwa & Muller, 2012; Motswainyana *et al.*, 2012). There is a detectable *trans* influence for the chloride anions, since the Pd1—Cl2 bond is significantly longer than Pd1—Cl1, thus reflecting the stronger *trans* influence of the diphenylphosphanyl group compared to the amine (Doherty *et al.*, 2002). The $Pd^{II}$ cation deviates by 0.0026 (3) Å from the best least-squares plane through atoms P1, N1, Cl1 and Cl2. This plane makes an angle of 46.57 (11)° with the best least-squares plane through the C2–C7 ring. The Pd-containing six-membered ring has a screw-boat confor-

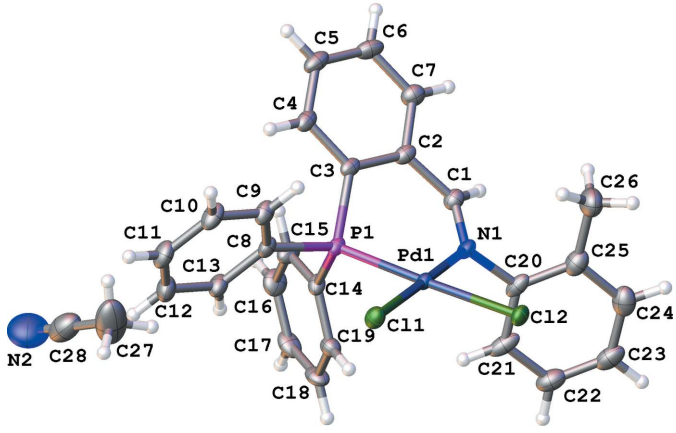



**Figure 1**
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

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mation, with atoms Pd1 and P1 deviating from the plane through the other four atoms.

Despite the presence of several benzene rings, no $\pi$–$\pi$ interactions are present in (I); only a number of weaker C—H···$\pi$ contacts are observed [C23—H23···$Cg1^{i}$ = 2.84 Å and C26—H26$A$···$Cg2^{ii}$ = 2.93 Å; $Cg1$ and $Cg2$ are the centroids of the C2–C7 and C14–C19 rings, respectively; symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$].

The asymmetric unit of (I) contains one acetonitrile solvent molecule, which was essential during the crystallization experiments to obtain good quality crystals. Two acetonitrile molecules occupy relatively large voids of 233 Å$^3$, and there are four such voids in the unit cell. In the packing, the position of the acetonitrile is fixed on one side by a C27—H27$C$···Cl2 interaction [H27$C$···Cl2$^{iii}$ = 2.70 Å; symmetry code: (iii) $-x+1, -y+2, -z+1$] and by a weak $\pi$-interaction (C27—H27$B$···$Cg2$ = 3.29 Å) (Fig. 2). Furthermore, atom N2 interacts with atoms H11, H16 and H22 of neighbouring molecules [N2···H11$^{iv}$ = 2.76 Å, N2···H16$^{v}$ = 2.65 Å and N2···H22$^{vi}$ = 2.78 Å; symmetry codes: (iv) $x, y-1, z$; (v) $-x+1, y, -z+\frac{1}{2}$; (vi) $-x+1, -y+1, -z+1$]. Despite these interactions, the acetonitrile molecules show a slight disorder, as indicated by the difference electron-density map (*e.g.* peaks of 0.63, 0.46 and −0.52 e Å$^{-3}$ close to acetonitrile).

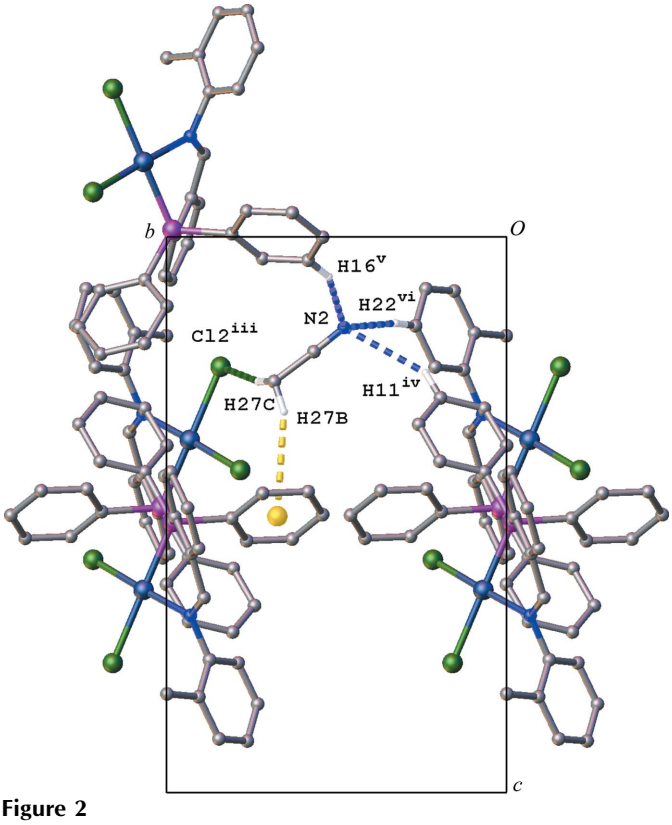


**Figure 2**
The interaction of the acetonitrile solvent molecules with neighbouring complex molecules in (I). Dashed lines indicate the various interactions. The centroid of the C14–C19 ring is indicated by a solid dot (yellow in the electronic version of the paper). For clarity, only H atoms involved in the interactions are shown. [Symmetry codes: (iii) $-x+1, -y+2, -z+1$; (iv) $x, y-1, z$; (v) $-x+1, y, -z+\frac{1}{2}$; (vi) $-x+1, -y+1, -z+1$.]

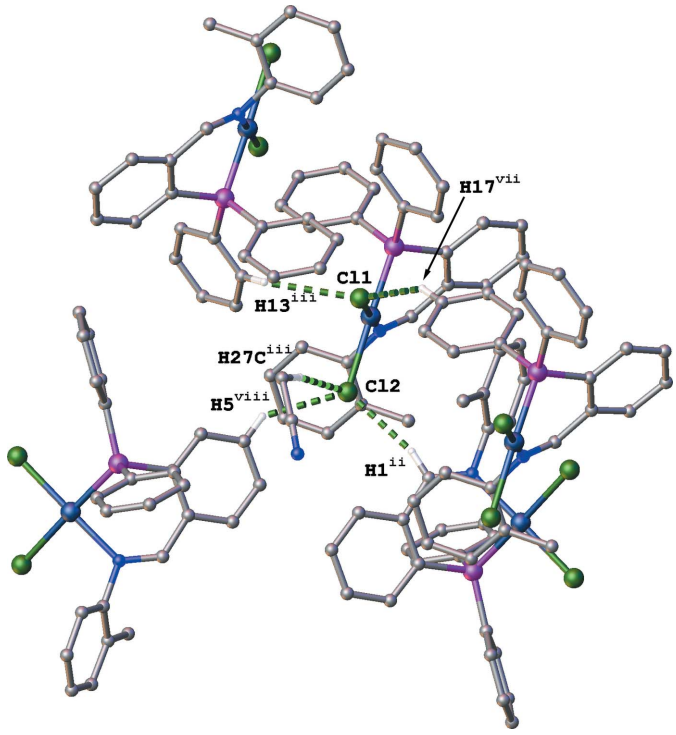


**Figure 3**
C—H···Cl interations (dashed lines) in the crystal packing of (I). For clarity, only H atoms involved in the interactions are shown. [Symmetry codes: (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+1, -y+2, -z+1$; (vii) $x, y+1, z$; (viii) $x, -y+2, z+\frac{1}{2}$.]

The shortest interactions for both Cl atoms are of the C—H···Cl type (Fig. 3) [Cl1···H13$^{iii}$ = 2.86 Å, Cl1···H17$^{vii}$ = 2.75 Å, Cl2···H1$^{ii}$ = 2.60 Å, Cl2···H5$^{viii}$ = 2.83 Å and Cl2···H27$C^{iii}$ = 2.70 Å; symmetry codes: (vii) $x, y+1, z$; (viii) $x, -y+2, z+\frac{1}{2}$].

The Cambridge Structural Database (CSD, Version 5.34; Allen, 2002) has 18 structures containing dichlorido-{[2-(diphenylphosphanyl)benzylidene]amine}palladium(II) groups. The angle between the best planes through the benzene ring and the $PdCl_2NP$ group range from 27.6 to 62.5°. The structure with refcode XUWHIG (Koprowski *et al.*, 2002) is almost identical to (I), only missing the *ortho*-methyl group, but crystallizes in the space group $P\overline{1}$. A fit of the Pd complex from the two structures, excluding the methyl group of (I), results in an r.m.s. deviation of 0.263 Å. As in (I), both Cl atoms attached to Pd also interact with H—C bonds. However, the interaction of the Cl atom in XUWHIG equivalent to Cl2 in (I) with the H atom in XUWHIG attached to the C atom equivalent to C25 in (I) results in the formation of centrosymmetric dimers in XUWHIG and hence in a different crystal packing compared to (I).

## Experimental

All reactions were carried out under a nitrogen atmosphere using a dual vacuum/nitrogen line and standard Schlenk techniques. Solvents were dried and purified by heating under reflux and under a nitrogen atmosphere in the presence of a suitable drying agent.

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Pd1—Cl1 | 2.2770 (7) | Pd1—P1 | 2.2122 (8) |
| Pd1—Cl2 | 2.3664 (7) | Pd1—N1 | 2.049 (2) |
| Cl1—Pd1—Cl2 | 89.95 (3) | N1—Pd1—Cl1 | 178.15 (7) |
| P1—Pd1—Cl1 | 91.45 (3) | N1—Pd1—Cl2 | 91.61 (7) |
| P1—Pd1—Cl2 | 178.15 (3) | N1—Pd1—P1 | 87.01 (7) |

For the preparation of *N*-[2-(diphenylphosphanyl)benzylidene]-2-methylaniline, 2-methylaniline (0.1030 g, 0.961 mmol) was added dropwise to a solution of 2-(diphenylphosphanyl)benzaldehyde (0.2790 g, 0.961 mmol) in dry $CH_2Cl_2$ (10 ml). Anhydrous magnesium sulfate (0.5 g) was added to the solution, after which the reaction was stirred at room temperature for 20 h. The resulting yellow mixture was filtered to obtain a yellow solution, which gave a yellow oil upon evaporation of the solvent (yield: 0.2990 g, 82%). IR (Nujol, $\nu$, $cm^{-1}$): 1622 (C═N imine), 1593, 1585, 1505 (C═C phenyl), 1435 (P—Ph). Analysis calculated for $C_{26}H_{22}NP$: C 82.30, H 5.84, N 3.69%; found: C 82.04, H 5.93, N 3.55%.

The preparation of (I) followed the synthetic protocol of Koprowski *et al.* (2002), with minor modifications at the precipitation stage of the product. Crystals of (I) suitable for X-ray crystallographic analysis were grown by slow evaporation from an acetonitrile solution of the complex (yield: 0.0697 g, 75%). IR (Nujol, $\nu$, $cm^{-1}$): 1614 (C═N imine), 1585, 1560, 1502 (C═C phenyl). Analysis calculated for $C_{26}H_{22}Cl_2NPPd$: C 56.09, H 3.98, N 2.52%; found: C 55.83, H 4.22, N 2.77%.

*Crystal data*

$[PdCl_2(C_{26}H_{22}NP)]\cdot C_2H_3N$
$M_r$ = 597.77
Monoclinic, $C2/c$
$a$ = 32.350 (3) Å
$b$ = 9.9963 (3) Å
$c$ = 20.8851 (16) Å
$\beta$ = 128.423 (13)°
$V$ = 5291.3 (12) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.98 $mm^{-1}$
$T$ = 100 K
0.2 × 0.2 × 0.2 mm

*Data collection*

Agilent SuperNova diffractometer (single source at offset, Eos detector)
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.983, $T_{max}$ = 1.000
10592 measured reflections
5391 independent reflections
4721 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.075
$S$ = 1.05
5391 reflections
309 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.75 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.52 e Å$^{-3}$

All H atoms were placed in idealized positions and refined in riding mode, with C—H = 0.93 (aromatic) or 0.96 Å (methyl) and $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

The authors acknowledge the University of the Western Cape Senate Research, the South African National Research Foundation and KU Leuven International Admissions and Mobility for financial support. The authors also thank the Hercules Foundation for supporting the purchase of the diffractometer through project No. AKUL/09/0035.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK3474). Services for accessing these data are described at the back of the journal.

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# supplementary materials

*Acta Cryst.* (2013). C**69** [doi:10.1107/S0108270113002333]

## Dichlorido{*N*-[2-(diphenylphosphanyl)benzylidene]-2-methyl-aniline}palladium(II) acetonitrile monosolvate

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*Crystal data*

$[PdCl_2(C_{26}H_{22}NP)]\cdot C_2H_3N$
$M_r$ = 597.77
Monoclinic, *C*2/*c*
*a* = 32.350 (3) Å
*b* = 9.9963 (3) Å
*c* = 20.8851 (16) Å
*β* = 128.423 (13)°
*V* = 5291.3 (12) Å$^3$
*Z* = 8
*F*(000) = 2416
$D_x$ = 1.501 Mg m$^{-3}$
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5198 reflections
*θ* = 2.9–26.3°
*μ* = 0.98 mm$^{-1}$
*T* = 100 K
Block, yellow
0.2 × 0.2 × 0.2 mm

*Data collection*

Agilent SuperNova diffractometer (single source at offset, Eos detector)
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 15.9631 pixels mm$^{-1}$
*ω* scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.983, $T_{max}$ = 1.000
10592 measured reflections
5391 independent reflections
4721 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025
$\theta_{max}$ = 26.4°, $\theta_{min}$ = 2.9°
*h* = −40→34
*k* = −12→10
*l* = −26→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.075
*S* = 1.05
5391 reflections
309 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
$w = 1/[\sigma^2(F_o^2) + (0.0255P)^2 + 11.5559P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.75 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.52 e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Pd1 | 0.637890 (8) | 1.06809 (2) | 0.634944 (12) | 0.01449 (7) |
| Cl1 | 0.57031 (3) | 1.21650 (7) | 0.58060 (4) | 0.02303 (16) |
| Cl2 | 0.67864 (3) | 1.15859 (7) | 0.76645 (4) | 0.02010 (15) |
| P1 | 0.60233 (3) | 0.98303 (7) | 0.51296 (4) | 0.01688 (15) |
| N1 | 0.69700 (9) | 0.9302 (2) | 0.68102 (13) | 0.0183 (5) |
| N2 | 0.38905 (17) | 0.4779 (4) | 0.1631 (3) | 0.0693 (11) |
| C1 | 0.71814 (11) | 0.8903 (3) | 0.64898 (17) | 0.0209 (6) |
| H1 | 0.7460 | 0.8304 | 0.6799 | 0.025* |
| C2 | 0.70380 (11) | 0.9276 (3) | 0.56977 (17) | 0.0201 (6) |
| C3 | 0.65416 (11) | 0.9765 (3) | 0.50325 (16) | 0.0182 (6) |
| C4 | 0.64503 (12) | 1.0060 (3) | 0.43027 (17) | 0.0222 (6) |
| H4 | 0.6121 | 1.0377 | 0.3860 | 0.027* |
| C5 | 0.68440 (12) | 0.9886 (3) | 0.42290 (18) | 0.0266 (7) |
| H5 | 0.6781 | 1.0107 | 0.3743 | 0.032* |
| C6 | 0.73281 (13) | 0.9387 (3) | 0.4874 (2) | 0.0282 (7) |
| H6 | 0.7591 | 0.9268 | 0.4822 | 0.034* |
| C7 | 0.74248 (12) | 0.9062 (3) | 0.56015 (19) | 0.0251 (7) |
| H7 | 0.7749 | 0.8700 | 0.6029 | 0.030* |
| C8 | 0.54572 (11) | 1.0641 (3) | 0.42268 (16) | 0.0198 (6) |
| C9 | 0.54967 (12) | 1.1958 (3) | 0.40363 (17) | 0.0243 (6) |
| H9 | 0.5818 | 1.2404 | 0.4357 | 0.029* |
| C10 | 0.50546 (12) | 1.2584 (3) | 0.33696 (18) | 0.0285 (7) |
| H10 | 0.5082 | 1.3451 | 0.3237 | 0.034* |
| C11 | 0.45714 (12) | 1.1941 (3) | 0.28948 (18) | 0.0302 (7) |
| H11 | 0.4276 | 1.2377 | 0.2449 | 0.036* |
| C12 | 0.45293 (13) | 1.0648 (3) | 0.30838 (18) | 0.0304 (7) |
| H12 | 0.4205 | 1.0214 | 0.2765 | 0.036* |
| C13 | 0.49723 (11) | 0.9997 (3) | 0.37519 (17) | 0.0250 (6) |
| H13 | 0.4943 | 0.9128 | 0.3880 | 0.030* |
| C14 | 0.58476 (10) | 0.8086 (3) | 0.50583 (16) | 0.0190 (6) |
| C15 | 0.59009 (12) | 0.7175 (3) | 0.46123 (18) | 0.0266 (7) |
| H15 | 0.6022 | 0.7464 | 0.4332 | 0.032* |
| C16 | 0.57752 (12) | 0.5837 (3) | 0.4580 (2) | 0.0305 (7) |
| H16 | 0.5813 | 0.5231 | 0.4282 | 0.037* |
| C17 | 0.55932 (11) | 0.5412 (3) | 0.4995 (2) | 0.0300 (7) |
| H17 | 0.5509 | 0.4516 | 0.4977 | 0.036* |
| C18 | 0.55362 (11) | 0.6306 (3) | 0.54345 (19) | 0.0272 (7) |

| | | | | |
|---|---|---|---|---|
| H18 | 0.5415 | 0.6011 | 0.5713 | 0.033* |
| C19 | 0.56584 (10) | 0.7646 (3) | 0.54659 (17) | 0.0225 (6) |
| H19 | 0.5614 | 0.8249 | 0.5758 | 0.027* |
| C20 | 0.71923 (12) | 0.8740 (3) | 0.76071 (17) | 0.0239 (6) |
| C21 | 0.68644 (14) | 0.7899 (3) | 0.7662 (2) | 0.0311 (7) |
| H21 | 0.6518 | 0.7735 | 0.7203 | 0.037* |
| C22 | 0.70622 (14) | 0.7324 (3) | 0.8402 (2) | 0.0330 (8) |
| H22 | 0.6857 | 0.6743 | 0.8447 | 0.040* |
| C23 | 0.75659 (14) | 0.7626 (3) | 0.9067 (2) | 0.0333 (8) |
| H23 | 0.7698 | 0.7247 | 0.9568 | 0.040* |
| C24 | 0.78840 (13) | 0.8462 (3) | 0.9028 (2) | 0.0347 (8) |
| H24 | 0.8224 | 0.8643 | 0.9497 | 0.042* |
| C25 | 0.76964 (13) | 0.9056 (3) | 0.82715 (19) | 0.0299 (7) |
| C26 | 0.80273 (13) | 0.9990 (4) | 0.8220 (2) | 0.0422 (9) |
| H26A | 0.8274 | 1.0419 | 0.8740 | 0.063* |
| H26B | 0.7807 | 1.0654 | 0.7811 | 0.063* |
| H26C | 0.8216 | 0.9506 | 0.8077 | 0.063* |
| C27 | 0.43269 (18) | 0.6835 (6) | 0.2598 (3) | 0.0827 (17) |
| H27A | 0.4461 | 0.7419 | 0.2401 | 0.124* |
| H27B | 0.4612 | 0.6549 | 0.3143 | 0.124* |
| H27C | 0.4069 | 0.7302 | 0.2602 | 0.124* |
| C28 | 0.40812 (17) | 0.5665 (5) | 0.2063 (3) | 0.0509 (11) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Pd1 | 0.01842 (11) | 0.01280 (11) | 0.01271 (11) | −0.00138 (8) | 0.00990 (9) | 0.00025 (8) |
| Cl1 | 0.0241 (3) | 0.0242 (4) | 0.0199 (3) | 0.0057 (3) | 0.0132 (3) | 0.0033 (3) |
| Cl2 | 0.0244 (3) | 0.0203 (3) | 0.0149 (3) | −0.0019 (3) | 0.0119 (3) | −0.0026 (3) |
| P1 | 0.0232 (4) | 0.0133 (3) | 0.0138 (3) | −0.0027 (3) | 0.0113 (3) | −0.0001 (3) |
| N1 | 0.0247 (12) | 0.0167 (12) | 0.0152 (11) | 0.0030 (10) | 0.0132 (10) | 0.0034 (10) |
| N2 | 0.085 (3) | 0.047 (2) | 0.088 (3) | −0.005 (2) | 0.059 (3) | 0.010 (2) |
| C1 | 0.0255 (15) | 0.0170 (14) | 0.0201 (14) | 0.0008 (12) | 0.0141 (12) | 0.0020 (12) |
| C2 | 0.0300 (15) | 0.0140 (13) | 0.0219 (14) | 0.0000 (12) | 0.0188 (13) | 0.0007 (12) |
| C3 | 0.0270 (14) | 0.0127 (13) | 0.0183 (13) | −0.0046 (12) | 0.0158 (12) | −0.0032 (11) |
| C4 | 0.0319 (16) | 0.0167 (14) | 0.0188 (14) | −0.0067 (13) | 0.0161 (13) | −0.0030 (12) |
| C5 | 0.0443 (18) | 0.0191 (15) | 0.0255 (15) | −0.0054 (14) | 0.0262 (15) | −0.0023 (13) |
| C6 | 0.0436 (18) | 0.0222 (16) | 0.0367 (18) | −0.0007 (15) | 0.0337 (16) | −0.0014 (14) |
| C7 | 0.0315 (16) | 0.0209 (15) | 0.0278 (16) | 0.0005 (13) | 0.0208 (14) | −0.0009 (13) |
| C8 | 0.0250 (14) | 0.0198 (14) | 0.0142 (13) | 0.0004 (13) | 0.0121 (12) | −0.0005 (12) |
| C9 | 0.0327 (16) | 0.0181 (14) | 0.0183 (14) | −0.0020 (13) | 0.0139 (13) | −0.0010 (12) |
| C10 | 0.0425 (18) | 0.0190 (15) | 0.0212 (15) | 0.0021 (14) | 0.0184 (14) | 0.0041 (13) |
| C11 | 0.0360 (17) | 0.0286 (17) | 0.0190 (15) | 0.0066 (15) | 0.0136 (14) | 0.0056 (14) |
| C12 | 0.0297 (16) | 0.0340 (18) | 0.0190 (15) | −0.0027 (15) | 0.0110 (13) | 0.0000 (14) |
| C13 | 0.0292 (15) | 0.0239 (16) | 0.0178 (14) | −0.0033 (14) | 0.0126 (13) | 0.0024 (13) |
| C14 | 0.0215 (14) | 0.0148 (13) | 0.0149 (13) | −0.0029 (12) | 0.0084 (11) | 0.0012 (11) |
| C15 | 0.0365 (17) | 0.0215 (16) | 0.0249 (15) | −0.0097 (14) | 0.0206 (14) | −0.0053 (13) |
| C16 | 0.0365 (18) | 0.0190 (16) | 0.0305 (17) | −0.0061 (14) | 0.0182 (15) | −0.0060 (13) |
| C17 | 0.0239 (15) | 0.0174 (15) | 0.0356 (18) | −0.0053 (13) | 0.0119 (14) | 0.0033 (14) |
| C18 | 0.0222 (15) | 0.0258 (16) | 0.0325 (17) | −0.0045 (13) | 0.0165 (14) | 0.0077 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C19 | 0.0187 (14) | 0.0234 (15) | 0.0237 (15) | −0.0009 (12) | 0.0123 (12) | 0.0024 (13) |
| C20 | 0.0359 (16) | 0.0209 (15) | 0.0209 (14) | 0.0131 (14) | 0.0207 (14) | 0.0075 (13) |
| C21 | 0.057 (2) | 0.0197 (15) | 0.0364 (18) | 0.0144 (16) | 0.0385 (17) | 0.0108 (14) |
| C22 | 0.047 (2) | 0.0278 (17) | 0.0385 (19) | 0.0070 (16) | 0.0337 (17) | 0.0076 (15) |
| C23 | 0.050 (2) | 0.0295 (18) | 0.0346 (18) | 0.0129 (16) | 0.0332 (17) | 0.0081 (15) |
| C24 | 0.0313 (17) | 0.0335 (19) | 0.0304 (17) | 0.0083 (16) | 0.0147 (15) | −0.0006 (15) |
| C25 | 0.0364 (17) | 0.0268 (17) | 0.0262 (16) | 0.0079 (15) | 0.0192 (15) | 0.0049 (14) |
| C26 | 0.0329 (18) | 0.052 (2) | 0.0304 (18) | 0.0002 (18) | 0.0141 (15) | 0.0054 (18) |
| C27 | 0.060 (3) | 0.119 (5) | 0.056 (3) | 0.019 (3) | 0.030 (2) | −0.028 (3) |
| C28 | 0.056 (3) | 0.063 (3) | 0.044 (2) | 0.019 (2) | 0.036 (2) | 0.015 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Pd1—Cl1 | 2.2770 (7) | C12—C13 | 1.393 (4) |
| Pd1—Cl2 | 2.3664 (7) | C13—H13 | 0.9300 |
| Pd1—P1 | 2.2122 (8) | C14—C15 | 1.388 (4) |
| Pd1—N1 | 2.049 (2) | C14—C19 | 1.393 (4) |
| P1—C3 | 1.811 (3) | C15—H15 | 0.9300 |
| P1—C8 | 1.809 (3) | C15—C16 | 1.387 (4) |
| P1—C14 | 1.811 (3) | C16—H16 | 0.9300 |
| N1—C1 | 1.282 (3) | C16—C17 | 1.383 (4) |
| N1—C20 | 1.454 (3) | C17—H17 | 0.9300 |
| N2—C28 | 1.134 (5) | C17—C18 | 1.373 (5) |
| C1—H1 | 0.9300 | C18—H18 | 0.9300 |
| C1—C2 | 1.462 (4) | C18—C19 | 1.386 (4) |
| C2—C3 | 1.405 (4) | C19—H19 | 0.9300 |
| C2—C7 | 1.402 (4) | C20—C21 | 1.413 (4) |
| C3—C4 | 1.392 (4) | C20—C25 | 1.368 (4) |
| C4—H4 | 0.9300 | C21—H21 | 0.9300 |
| C4—C5 | 1.385 (4) | C21—C22 | 1.378 (4) |
| C5—H5 | 0.9300 | C22—H22 | 0.9300 |
| C5—C6 | 1.376 (4) | C22—C23 | 1.365 (5) |
| C6—H6 | 0.9300 | C23—H23 | 0.9300 |
| C6—C7 | 1.386 (4) | C23—C24 | 1.367 (5) |
| C7—H7 | 0.9300 | C24—H24 | 0.9300 |
| C8—C9 | 1.404 (4) | C24—C25 | 1.422 (4) |
| C8—C13 | 1.387 (4) | C25—C26 | 1.474 (5) |
| C9—H9 | 0.9300 | C26—H26A | 0.9600 |
| C9—C10 | 1.379 (4) | C26—H26B | 0.9600 |
| C10—H10 | 0.9300 | C26—H26C | 0.9600 |
| C10—C11 | 1.383 (4) | C27—H27A | 0.9600 |
| C11—H11 | 0.9300 | C27—H27B | 0.9600 |
| C11—C12 | 1.382 (4) | C27—H27C | 0.9600 |
| C12—H12 | 0.9300 | C27—C28 | 1.464 (7) |
| | | | |
| Cl1—Pd1—Cl2 | 89.95 (3) | C11—C12—C13 | 120.0 (3) |
| P1—Pd1—Cl1 | 91.45 (3) | C13—C12—H12 | 120.0 |
| P1—Pd1—Cl2 | 178.15 (3) | C8—C13—C12 | 120.1 (3) |
| N1—Pd1—Cl1 | 178.15 (7) | C8—C13—H13 | 120.0 |
| N1—Pd1—Cl2 | 91.61 (7) | C12—C13—H13 | 120.0 |

| | | | |
|---|---|---|---|
| N1—Pd1—P1 | 87.01 (7) | C15—C14—P1 | 121.6 (2) |
| C3—P1—Pd1 | 106.73 (9) | C15—C14—C19 | 119.2 (3) |
| C3—P1—C14 | 102.78 (13) | C19—C14—P1 | 119.2 (2) |
| C8—P1—Pd1 | 119.56 (9) | C14—C15—H15 | 119.7 |
| C8—P1—C3 | 107.90 (13) | C16—C15—C14 | 120.7 (3) |
| C8—P1—C14 | 106.41 (13) | C16—C15—H15 | 119.7 |
| C14—P1—Pd1 | 112.13 (9) | C15—C16—H16 | 120.3 |
| C1—N1—Pd1 | 127.53 (19) | C17—C16—C15 | 119.5 (3) |
| C1—N1—C20 | 115.6 (2) | C17—C16—H16 | 120.3 |
| C20—N1—Pd1 | 116.78 (17) | C16—C17—H17 | 119.8 |
| N1—C1—H1 | 116.0 | C18—C17—C16 | 120.3 (3) |
| N1—C1—C2 | 127.9 (3) | C18—C17—H17 | 119.8 |
| C2—C1—H1 | 116.0 | C17—C18—H18 | 119.7 |
| C3—C2—C1 | 124.9 (3) | C17—C18—C19 | 120.5 (3) |
| C7—C2—C1 | 116.1 (3) | C19—C18—H18 | 119.7 |
| C7—C2—C3 | 119.0 (3) | C14—C19—H19 | 120.1 |
| C2—C3—P1 | 118.1 (2) | C18—C19—C14 | 119.8 (3) |
| C4—C3—P1 | 122.3 (2) | C18—C19—H19 | 120.1 |
| C4—C3—C2 | 119.4 (3) | C21—C20—N1 | 117.4 (3) |
| C3—C4—H4 | 119.6 | C25—C20—N1 | 120.1 (3) |
| C5—C4—C3 | 120.7 (3) | C25—C20—C21 | 122.5 (3) |
| C5—C4—H4 | 119.6 | C20—C21—H21 | 120.3 |
| C4—C5—H5 | 119.9 | C22—C21—C20 | 119.3 (3) |
| C6—C5—C4 | 120.1 (3) | C22—C21—H21 | 120.3 |
| C6—C5—H5 | 119.9 | C21—C22—H22 | 120.7 |
| C5—C6—H6 | 119.9 | C23—C22—C21 | 118.5 (3) |
| C5—C6—C7 | 120.1 (3) | C23—C22—H22 | 120.7 |
| C7—C6—H6 | 119.9 | C22—C23—H23 | 118.6 |
| C2—C7—H7 | 119.7 | C22—C23—C24 | 122.8 (3) |
| C6—C7—C2 | 120.5 (3) | C24—C23—H23 | 118.6 |
| C6—C7—H7 | 119.7 | C23—C24—H24 | 119.9 |
| C9—C8—P1 | 120.2 (2) | C23—C24—C25 | 120.3 (3) |
| C13—C8—P1 | 120.0 (2) | C25—C24—H24 | 119.9 |
| C13—C8—C9 | 119.6 (3) | C20—C25—C24 | 116.6 (3) |
| C8—C9—H9 | 120.3 | C20—C25—C26 | 122.3 (3) |
| C10—C9—C8 | 119.5 (3) | C24—C25—C26 | 121.1 (3) |
| C10—C9—H9 | 120.3 | H27A—C27—H27B | 109.5 |
| C9—C10—H10 | 119.5 | H27A—C27—H27C | 109.5 |
| C9—C10—C11 | 120.9 (3) | H27B—C27—H27C | 109.5 |
| C11—C10—H10 | 119.5 | C28—C27—H27A | 109.5 |
| C10—C11—H11 | 120.1 | C28—C27—H27B | 109.5 |
| C12—C11—C10 | 119.8 (3) | C28—C27—H27C | 109.5 |
| C12—C11—H11 | 120.1 | N2—C28—C27 | 178.0 (5) |
| C11—C12—H12 | 120.0 | | |

| | | | |
|---|---|---|---|
| Pd1—P1—C3—C2 | 45.0 (2) | C3—P1—C14—C15 | −29.3 (3) |
| Pd1—P1—C3—C4 | −141.1 (2) | C3—P1—C14—C19 | 150.1 (2) |
| Pd1—P1—C8—C9 | 61.7 (3) | C3—C2—C7—C6 | 3.0 (4) |
| Pd1—P1—C8—C13 | −113.7 (2) | C3—C4—C5—C6 | 1.5 (4) |

| | | | |
|---|---|---|---|
| Pd1—P1—C14—C15 | −143.6 (2) | C4—C5—C6—C7 | −0.3 (5) |
| Pd1—P1—C14—C19 | 35.9 (2) | C5—C6—C7—C2 | −2.0 (5) |
| Pd1—N1—C1—C2 | −3.4 (4) | C7—C2—C3—P1 | 172.3 (2) |
| Pd1—N1—C20—C21 | 68.0 (3) | C7—C2—C3—C4 | −1.8 (4) |
| Pd1—N1—C20—C25 | −110.6 (3) | C8—P1—C3—C2 | 174.7 (2) |
| Cl1—Pd1—P1—C3 | 131.11 (10) | C8—P1—C3—C4 | −11.4 (3) |
| Cl1—Pd1—P1—C8 | 8.46 (11) | C8—P1—C14—C15 | 84.0 (3) |
| Cl1—Pd1—P1—C14 | −117.09 (10) | C8—P1—C14—C19 | −96.6 (2) |
| Cl2—Pd1—N1—C1 | −140.8 (2) | C8—C9—C10—C11 | 1.1 (5) |
| Cl2—Pd1—N1—C20 | 36.6 (2) | C9—C8—C13—C12 | 0.9 (4) |
| P1—Pd1—N1—C1 | 37.9 (2) | C9—C10—C11—C12 | −0.6 (5) |
| P1—Pd1—N1—C20 | −144.6 (2) | C10—C11—C12—C13 | 0.1 (5) |
| P1—C3—C4—C5 | −174.3 (2) | C11—C12—C13—C8 | −0.3 (5) |
| P1—C8—C9—C10 | −176.7 (2) | C13—C8—C9—C10 | −1.3 (4) |
| P1—C8—C13—C12 | 176.3 (2) | C14—P1—C3—C2 | −73.1 (2) |
| P1—C14—C15—C16 | 178.6 (2) | C14—P1—C3—C4 | 100.7 (2) |
| P1—C14—C19—C18 | −178.2 (2) | C14—P1—C8—C9 | −170.1 (2) |
| N1—Pd1—P1—C3 | −49.93 (11) | C14—P1—C8—C13 | 14.5 (3) |
| N1—Pd1—P1—C8 | −172.58 (13) | C14—C15—C16—C17 | 0.2 (5) |
| N1—Pd1—P1—C14 | 61.88 (12) | C15—C14—C19—C18 | 1.2 (4) |
| N1—C1—C2—C3 | −23.0 (5) | C15—C16—C17—C18 | 0.1 (5) |
| N1—C1—C2—C7 | 159.9 (3) | C16—C17—C18—C19 | 0.2 (5) |
| N1—C20—C21—C22 | 178.7 (3) | C17—C18—C19—C14 | −0.9 (4) |
| N1—C20—C25—C24 | −179.9 (3) | C19—C14—C15—C16 | −0.9 (4) |
| N1—C20—C25—C26 | 1.8 (5) | C20—N1—C1—C2 | 179.1 (3) |
| C1—N1—C20—C21 | −114.3 (3) | C20—C21—C22—C23 | 2.2 (5) |
| C1—N1—C20—C25 | 67.2 (4) | C21—C20—C25—C24 | 1.7 (5) |
| C1—C2—C3—P1 | −4.7 (4) | C21—C20—C25—C26 | −176.7 (3) |
| C1—C2—C3—C4 | −178.7 (3) | C21—C22—C23—C24 | −0.8 (5) |
| C1—C2—C7—C6 | −179.8 (3) | C22—C23—C24—C25 | −0.3 (5) |
| C2—C3—C4—C5 | −0.5 (4) | C23—C24—C25—C20 | −0.1 (5) |
| C3—P1—C8—C9 | −60.4 (3) | C23—C24—C25—C26 | 178.2 (3) |
| C3—P1—C8—C13 | 124.2 (2) | C25—C20—C21—C22 | −2.7 (5) |