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trans-Dichlorobis(triphenylphosphine)-palladium(II) dichloroethane solvate

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.006 Å
R factor = 0.039
wR factor = 0.098
Data-to-parameter ratio = 19.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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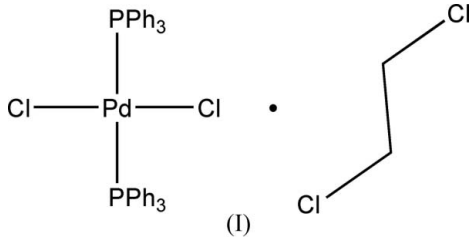
In the title compound, $[PdCl_2(C_{18}H_{15}P)_2]\cdot C_2H_4Cl_2$, the Pd-complex and dichloroethane solvent molecule both possess a crystallographicaly imposed centre of symmetry. A square planar geometry about the palladium(II) metal centre is observed, while the *trans* triphenylphosphine ligands are in an eclipsed conformation. The most important bond distances include Pd—P 2.3394 (13) Å and Pd—Cl 2.3255 (12) Å. No hydrogen bonding is observed in the crystal structure.

Comment

A range of crystal structures have been reported for *trans*-dichlorobis(triphenylphosphine)palladium(II) complexes, both with and without a solvent molecule (CSD; Version 5.27; Allen, 2002; Ferguson *et al.*, 1982; Kitano *et al.*, 1983; Oilunkaniemi *et al.*, 2003; Stark & Whitmire, 1997). The title compound, (I), is presented as an example of a dichloroethane solvate.



(I)

In (I), a square planar geometry about the palladium(II) metal centre is observed (Fig. 1). The Pd—P bond distances are nearly the same as those in the solvent-free complex (Ferguson *et al.*, 1982), while the Pd—Cl distances correspond to those observed in the dichloromethane solvate structure (Oilunkaniemi *et al.*, 2003). The triphenylphosphine units are in an eclipsed conformation about the palladium(II) centre, as evidenced by the Cl—Pd—P—C torsion angles (Table 1). The complex molecule and solvent molecule both lie on inversion centres (Fig. 2). No significant hydrogen bonds are found in (I).

Experimental

The title complex was synthesized by the addition of PPh_3 (83 mg, 0.316 mmol) to a dichloroethane (10 ml) solution of the bis-tribromotropolonatopalladium(II) complex (100 mg, 0.287 mmol). The suspension dissolved and gave an orange solution. On evaporation of the solvent, crystals suitable for X-ray crystallography were obtained (yield: 50 mg).

Crystal data

$[PdCl_2(C_{18}H_{15}P)_2]\cdot C_2H_4Cl_2$
$M_r = 800.81$
Triclinic, $P\overline{1}$
$a = 9.208$ (5) Å
$b = 9.481$ (5) Å
$c = 11.599$ (5) Å
$\alpha = 110.177$ (5)°
$\beta = 107.723$ (5)°
$\gamma = 98.921$ (5)°
$V = 866.2$ (8) Å^3
$Z = 1$
$D_x = 1.535$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.96$ mm^{-1}
$T = 100$ (2) K
Block, yellow
0.17 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.847$, $T_{max} = 0.905$
23018 measured reflections
3774 independent reflections
3487 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.099$
$S = 1.05$
3774 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 3.9311P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.99$ e Å^{-3}
$\Delta\rho_{min} = -1.41$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pd—Cl	2.3255 (12)	Pd—P	2.3394 (13)
Cl—Pd—P	88.03 (3)		
Cl—Pd—P—C11	−77.20 (12)	Cl—Pd—P—C31	163.86 (12)
Cl—Pd—P—C21	43.45 (12)		

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}$(parent atom). The maximal residual peak is 0.05 Å from Cl and the deepest hole 0.05 Å from the Pd atom.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2004); software used to prepare material for publication: *SHELXL97*.

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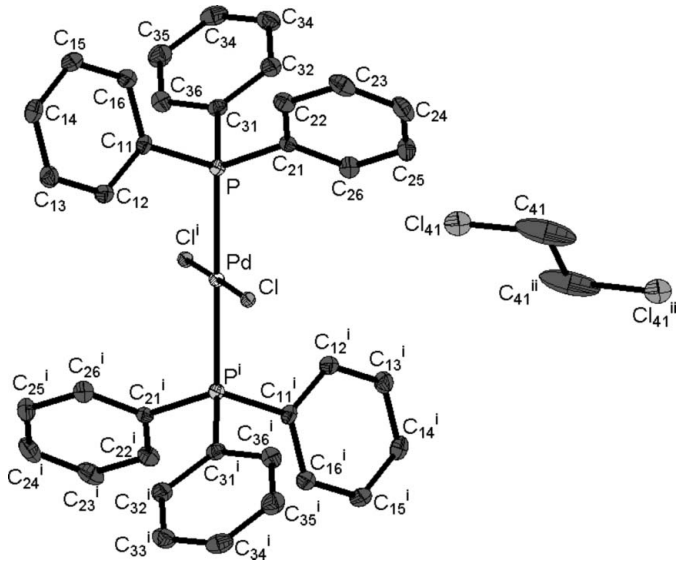

Figure 1
Representation of the title compound (I), showing the numbering scheme and 50% probability displacement ellipsoids. H atoms have been omitted for clarity. [Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $2-x, -y, 1-z$]

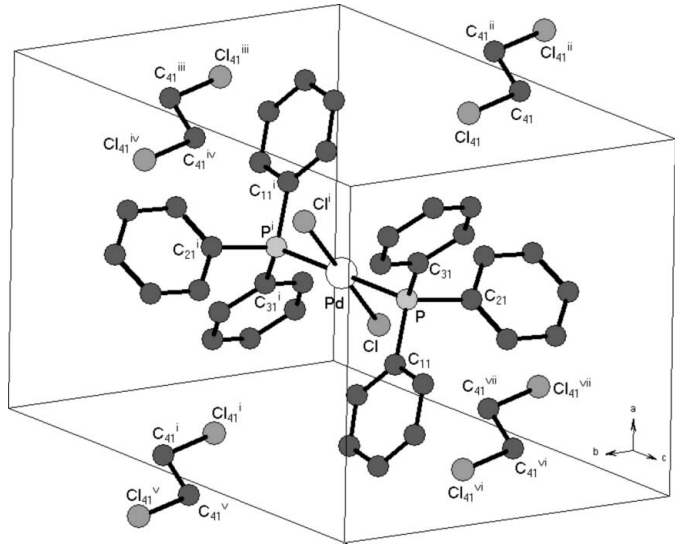

Figure 2
The packing of the complex and solvent molecules. H atoms have been omitted for clarity. [Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $2-x, -y, 1-z$; (iii) $2-x, 1-y, 1-z$; (iv) $x, 1+y, z$; (v) $-1+x, 1+y, z$; (vi) $-1+x, y, z$; (vii) $1-x, -y, 1-z$].

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