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Dichloro{1-[2-(diphenylphosphino-κ*P*)ethyl]-1,3-dihydro-3-(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene-κ*C*}palladium(II) diethyl ether solvate

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Key indicators

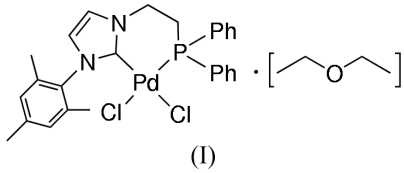
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.031
wR factor = 0.080
Data-to-parameter ratio = 20.3

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

The structure of the title compound, $[PdCl_2(C_{26}H_{27}N_2P)]\cdot C_4H_{10}O$, was determined at 150 K. The palladium center is in a square-planar coordination geometry. A non-classical hydrogen bond (C—H···O) exists between the palladium complex and solvent molecule. The two chloride ligands are also involved in weak non-classical hydrogen bonds linking two neighboring molecules.

Comment

Palladium complexes with bidentate phosphine-functionalized N-heterocyclic carbene (NHC) ligands have been demonstrated to be efficient in C—C coupling reactions (Yang *et al.*, 2001; Tsoureas *et al.*, 2003; Lee *et al.*, 2004). Several structures of these complexes have been determined by the last two groups. We report here the structure of dichloro{1-[2-(diphenylphosphino-κ*P*)ethyl]-1,3-dihydro-3-(2,4,6-trimethylphenyl)-2*H*-imidazol-2-ylidene-κ*C*}palladium(II) diethyl ether solvate, (I). The dibromopalladium analog, (II), was previously determined by Tsoureas *et al.* (2003).



(I)

The title compound, (I), crystallizes in the monoclinic space group $P2_1/c$ with the inclusion of a diethyl ether molecule in its asymmetric unit, whereas (II) crystallizes in the triclinic space group $P\overline{1}$ without solvent incorporation. The palladium center is in a square-planar coordination geometry. The Pd—Cl bond *trans* to P is longer than that *trans* to NHC by *ca* 0.02 Å. The Pd—C bond distance in (I) is identical to that in (II) [1.996 (3) Å], while the Pd—P bond in (I) is shorter [(I): 2.2287 (11) Å; (II): 2.2461 (7) Å].

The diethyl ether solvent molecule is involved in a non-classical hydrogen bond *via* the O atom with one of the imidazole ring H atoms of the palladium complex [C—H···O = 3.381 (4) Å]. The two chloride ligands are also involved in long non-classical hydrogen bonds with H atoms on the ethylene spacer and imidazole ring of a neigbouring molecule [C—H···Cl = 3.286 (3) and 3.772 (3) Å, respectively].

Experimental

The title compound was prepared according to the literature procedure of Lee *et al.* (2004). Suitable crystals were obtained by slow diffusion of diethyl ether into a dimethylformamide solution of the palladium complex at room temperature.

Crystal data

$[PdCl_2(C_{26}H_{27}N_2P)]\cdot C_4H_{10}O$	D_x = 1.432 Mg m^{-3}
M_r = 649.89	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 926 reflections
a = 13.046 (5) Å	θ = 2.9–26.9°
b = 14.242 (6) Å	μ = 0.87 mm^{-1}
c = 16.289 (7) Å	T = 150 (2) K
β = 95.01 (4)°	Plate, colorless
V = 3015 (2) Å^3	0.36 × 0.30 × 0.06 mm
Z = 4	

Data collection

Bruker SMART 1000 diffractometer	6845 independent reflections
	5422 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.033
Absorption correction: multi-scan (*SADABS*, Sheldrick, 2002)	θ_{max} = 27.5°
	$h = -16 \rightarrow 16$
T_{min} = 0.745, T_{max} = 0.950	$k = -18 \rightarrow 18$
29264 measured reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 2.9149P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.031	
$wR(F^2)$ = 0.080	
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.002
6845 reflections	$\Delta\rho_{max}$ = 0.77 e Å^{-3}
337 parameters	$\Delta\rho_{min}$ = −0.40 e Å^{-3}
H-atom parameters constrained	

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···Cl2^{i}	0.95	2.93	3.772 (3)	148
C3—H3A···O1	0.95	2.45	3.381 (4)	167
C5—H5A···Cl1^{i}	0.99	2.90	3.286 (3)	104

Symmetry code: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$.

All H atoms were positioned geometrically and refined with a riding model, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for all other H atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

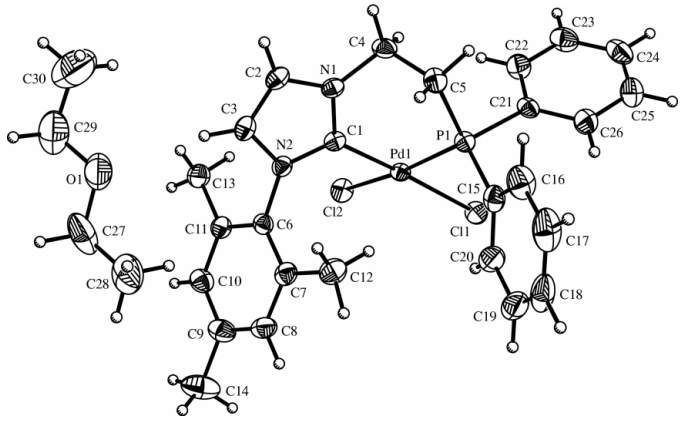


Figure 1
A view of the asymmetric unit, drawn with 50% displacement ellipsoids for non-H atoms.

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