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trans-Di-μ-chloro-bis[chloro(tricyclohexylphosphine)palladium] benzene solvate

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Key indicators

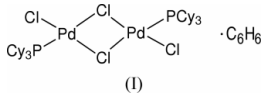
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.033
wR factor = 0.083
Data-to-parameter ratio = 19.7

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

The title compound, *trans*-$[Pd_2Cl_4(PCy_3)_2]\cdot C_6H_6$, where PCy_3 is tricyclohexylphosphine ($C_{18}H_{33}P$), cocrystallizes with one benzene molecule in the centrosymmetric space group $P2_1/c$ and both molecules lie on inversion centers. Each Pd atom adopts a distorted square-planar geometry [angles vary from 84.23 (3) to 95.82 (3)°], and is bonded to a terminal chloride, a phosphine and two bridging chlorides. Bond lengths are typical of related species.

Comment

The general class of $[PdCl_2P]_2$ complexes has been known since the early studies of Mann & Purdie (1935) and Mann & Wells (1938). The title complex, (I), was prepared as a precursor to other palladium complexes. The structures of a range of related palladium complexes have been determined (Chaloner *et al.*, 1995; Coles *et al.*, 1999; Grigsby & Nicholson, 1992; Vicente *et al.*, 1997), all presenting virtually the same structural parameters as those of the complex reported here.



(I)

Experimental

The title compound was isolated as a side-product of the reaction of $(PhCN)_2PdCl_2$ with indenyllithium and PCy_3. Single crystals suitable for X-ray diffraction study were obtained from a benzene solution.

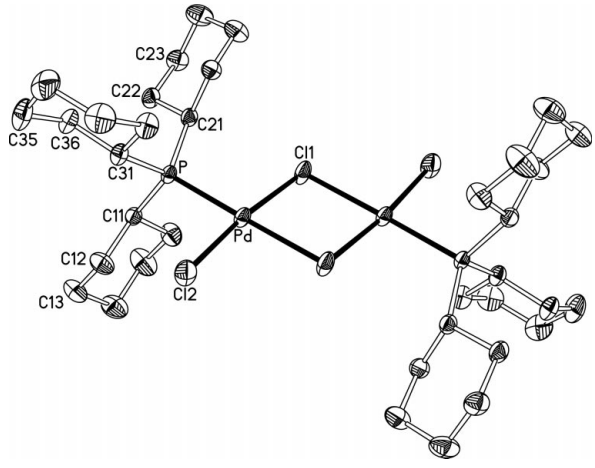


Figure 1
View of the title molecule. Ellipsoids correspond to 30% probability. The unlabeled part of the molecule is related by the symmetry transformation $(1-x, -y, 2-z)$.

Crystal data

$[Pd_2Cl_4(C_{18}H_{33}P)_2]\cdot C_6H_6$	D_x = 1.430 Mg m^{-3}
M_r = 993.58	Cu $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6051 reflections
a = 9.9954 (1) Å	θ = 2.7–72.5°
b = 16.463 (1) Å	μ = 9.27 mm^{-1}
c = 14.095 (1) Å	T = 293 (2) K
β = 95.657 (1)°	Block, light orange-red
V = 2308.1 (2) Å^3	0.16 × 0.14 × 0.08 mm
Z = 2	

Data collection

Bruker SMART 2K diffractometer	3791 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.063
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996*a*)	θ_{max} = 72.7°
T_{min} = 0.266, T_{max} = 0.475	$h = -9 \rightarrow 11$
27 337 measured reflections	$k = -20 \rightarrow 20$
4457 independent reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$w = 1/[\sigma^2(F_o^2) + (0.0525P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.083	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 0.42 e Å^{-3}
4457 reflections	$\Delta\rho_{min}$ = −0.57 e Å^{-3}
226 parameters	

Table 1
Selected geometric parameters (Å, °).

Pd—P	2.2495 (7)	Pd—Cl1	2.3217 (8)
Pd—Cl2	2.2862 (8)	Pd—Cl1^{i}	2.4370 (7)
P—Pd—Cl2	90.16 (3)	Cl2—Pd—Cl1^{i}	89.86 (3)
P—Pd—Cl1	95.82 (3)	Cl1—Pd—Cl1^{i}	84.23 (3)
Cl2—Pd—Cl1	173.53 (3)	Pd—Cl1—Pd^{i}	95.77 (3)
P—Pd—Cl1^{i}	178.32 (3)		
P—Pd—Cl1—Pd^{i}	178.31 (3)	Cl1—Pd—P—C31	−136.92 (11)
Cl1^{i}—Pd—Cl1—Pd^{i}	0	Cl2—Pd—P—C21	169.53 (11)
Cl2—Pd—P—C11	−73.97 (10)	Cl1—Pd—P—C21	−12.94 (11)
Cl1—Pd—P—C11	103.56 (10)	C21—P—C31—C32	−78.0 (3)
Cl2—Pd—P—C31	45.55 (11)	Pd—P—C31—C32	45.7 (3)

Symmetry code: (i) $1-x, -y, 2-z$.

H atoms were constrained to the parent site using a riding model, with *SHELXL*96 (Sheldrick, 1996*b*) defaults (C—H = 0.94 Å). U_{iso}(H) values were set at $1.2U_{eq}$ of the parent C atoms. A final verification of possible voids was performed using the VOID routine of the *PLATON* program (Spek, 1995).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*96 (Sheldrick, 1996*b*); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL*96.

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