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trans-Dichloro{*P*,*P*′-[3,3′-oxybis(*m*-phenylenemethylene)]bis(diphenylphosphine)}palladium(II)

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Key indicators

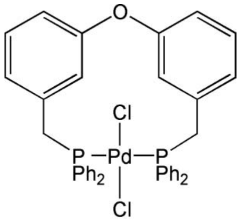
Single-crystal X-ray study
T = 203 K
Mean σ(C–C) = 0.006 Å
R factor = 0.037
wR factor = 0.074
Data-to-parameter ratio = 16.1

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

The square-planar title complex, [$PdCl_2(C_{38}H_{32}OP_2)$], shows the P atoms to be *trans* coordinated, with a P—Pd—P angle of 176.50 (4)°. The phenyl rings in the phosphorus ligand are inclined at an angle of 61.2 (1)° to each other.

Comment

Square-planar complexes of palladium(II) have long been recognized to play a central role in catalytic reactions (Cornils & Herrmann, 1996). Recently, we studied the catalytic activity of *trans*-palladium complexes in Suzuki cross-coupling reactions. For comparison, we have synthesized the title compound, (I). Although it has been known for almost 20 years (Marty *et al.*, 1987), its structure has never been solved by X-ray structure analysis.



(I)

The single-crystal X-ray structure analysis of (I) shows the Pd atom to be in a square-planar geometry, surrounded by two Cl and two P atoms (Fig. 1). The chelating diphosphine ligand adopts a *trans* coordination geometry. Despite the formation of a 12-membered chelate ring, the distortion imposed around the Pd atom is negligible. The P—Pd—P angle [176.50 (4)°] is almost 180°, as expected for *trans* coordination. Atoms Pd1, P1, P2, Cl1 and Cl2 are essentially coplanar, with an average deviation from planarity of 0.0345 Å. Selected bond lengths and angles for (I) are listed in Table 1, and are very similar to that of the $PtBr_2$ analogous complex [$PtBr_2(C_{38}H_{32}OP_2)$] (Stoeckli-Evans *et al.*, 1987). The two C_6H_4 planes of the 3,3′-oxydibenzyl ligand are inclined at an angle of 61.2 (1)° to each other. The C—O—C angle is 120.3 (3)°.

In the crystal structure, the molecules exist as dimers due to the presence of weak intermolecular interactions between a CH_2 proton and the Cl atom of a neighbouring molecule. (Table 2).

Experimental

Compound (I) was prepared according to the published method of Marty *et al.* (1987). Crystals were obtained by slow evaporation of a chloroform solution.

Crystal data

$[PdCl_2(C_{38}H_{32}OP_2)]$
$M_r = 743.88$
Orthorhombic, *Pbca*
$a = 11.4170\ (5)$ Å
$b = 20.8796\ (17)$ Å
$c = 27.6747\ (13)$ Å
$V = 6597.2\ (7)$ Å^3
$Z = 8$
$D_x = 1.498$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.85$ mm^{-1}
$T = 203\ (2)$ K
Plate, orange
0.28 × 0.16 × 0.08 mm

Data collection

Stoe IPDS diffractometer
φ scans
Absorption correction: none
24892 measured reflections
6403 independent reflections
3612 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.073$
$\theta_{\rm max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.074$
$S = 0.82$
6403 reflections
397 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.64$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.80$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—P1	1.835 (4)	P1—Pd1	2.3341 (11)
C6—O1	1.396 (5)	P2—Pd1	2.3275 (10)
C8—O1	1.388 (5)	Cl1—Pd1	2.3034 (9)
C14—P2	1.843 (4)	Cl2—Pd1	2.2916 (9)
C8—O1—C6	120.3 (3)	Cl2—Pd1—Cl1	179.21 (4)
C1—P1—Pd1	110.35 (14)	P2—Pd1—P1	176.50 (4)
C14—P2—Pd1	113.97 (13)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*B*···Cl2	0.97	3.09	3.565 (4)	112

All H atoms were placed in calculated positions (C—H = 0.93 Å for CH and 0.97 Å for CH$_2$) and treated as riding atoms with the constraint $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(carrier) applied.

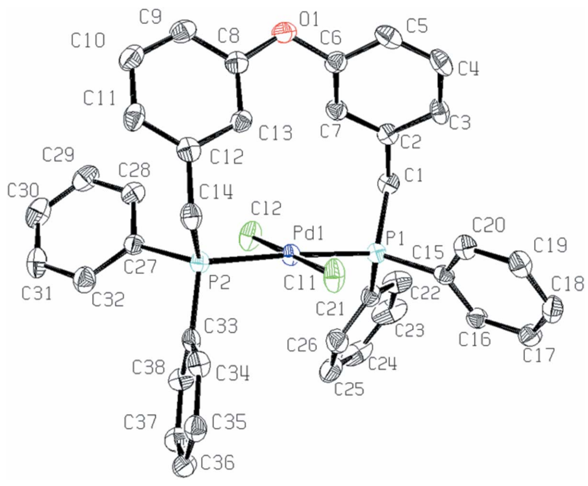


Figure 1
The molecular structure of (I) with the H atoms omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

Data collection: *EXPOSE* in *IPDS Software* Software Software (Stoe & Cie, 2000); cell refinement: *CELL* in *IPDS Software* Software Software; data reduction: *INTEGRATE* in *IPDS Software* Software Software; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-32* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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