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cis-Dichlorobis(triphenyphosphite-*P*)-palladium(II)

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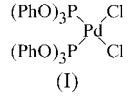
In the title compound, $[PdCl_2\{P(OPh)_3\}_2]$, the Pd^{II} centre shows slightly distorted square-planar geometry, with the two chloro ligands in *cis* positions.

Comment

During a study of the substitution reactions of $[PdCl_2\{P(OPh)_3\}_2]$, (I), we noticed that there is no reported X-ray structure determination of this complex. This was due to difficulty experienced in crystallizing the compound from the ethanol reaction solution (Ahmed *et al.*, 1973). IR and NMR data of the compound are in agreement with an earlier conclusion (Allen *et al.*, 1970). With new X-ray data, it is now clear that Pd^{II} adopts a distorted four-coordinate geometry involving two chloro ligands and two phosphite groups. Evidently, the Cl1—Pd—Cl2 [90.74 (4)°] and P1—Pd—P2 [98.15 (4)°] angles are wider than their ideal values of 90° due to bulky phosphite ligands. The Cl1—Pd—Cl2 angle is also narrower than the P1—Pd—P2 angle, and this is apparently due to steric effects of the phosphite ligands. The Pd—P and Pd—Cl bonds are approximately within the same range of other phosphine complexes (Kitano & Ashida, 1983; Ferguson *et al.*, 1982).



(I)

Experimental

The title complex was prepared by refluxing $[PdCl_4]^{2-}$ and $P(OPh_3)$ in a molar ratio of 1:2 in toluene for 6 h. The yellow precipitate was extracted from the resultant suspension and colourless crystals suitable for X-ray diffraction analysis were obtained by slow addition of methanol into a solution of the compound in chloroform. Since our values of δ_p and ^1J(Pd–P) are in excellent agreement with those in the literature (Ahmed *et al.*, 1973), they are not reproduced here.

Crystal data

$[PdCl_2(C_{18}H_{15}O_3P)_2]$	D_x = 1.548 Mg m^{-3}
M_r = 797.90	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 5000 reflections
a = 9.2007 (9) Å	θ = 2.13–26.14°
b = 12.2973 (17) Å	μ = 0.837 mm^{-1}
c = 30.421 (3) Å	T = 213 (2) K
β = 93.260 (12)°	Plate, colourless
V = 3436.4 (7) Å^3	0.28 × 0.16 × 0.12 mm
Z = 4	

Data collection

Stoe IPDS diffractometer	4139 reflections with $I > 2\sigma(I)$
Image plate scans	R_{int} = 0.091
Absorption correction: numerical (*X-SHAPE*; Stoe, 1997)	θ_{max} = 26.14°
T_{min} = 0.818, T_{max} = 0.916	$h = -11 \rightarrow 11$
26 396 measured reflections	$k = -15 \rightarrow 15$
6755 independent reflections	$l = -37 \rightarrow 37$

Refinement

Refinement on F^2	H-atom parameters constrained
$R(F)$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.107	$(\Delta/\sigma)_{max}$ = 0.002
S = 0.861	$\Delta\rho_{max}$ = 0.97 e Å^{-3}
6755 reflections	$\Delta\rho_{min}$ = −1.30 e Å^{-3}
424 parameters	

Table 1
Selected geometric parameters (Å, °).

O1—P1	1.583 (3)	O6—P2	1.584 (3)
O2—P1	1.585 (3)	P1—Pd1	2.2299 (11)
O3—P1	1.588 (3)	P2—Pd1	2.2314 (12)
O4—P2	1.580 (3)	Cl1—Pd1	2.3273 (11)
O5—P2	1.584 (3)	Cl2—Pd1	2.3354 (11)
O1—P1—O2	94.12 (16)	O4—P2—Pd1	118.29 (12)
O1—P1—O3	108.35 (16)	O5—P2—Pd1	113.44 (12)
O2—P1—O3	104.66 (16)	O6—P2—Pd1	115.38 (12)
O1—P1—Pd1	114.54 (12)	P1—Pd1—P2	98.15 (4)
O2—P1—Pd1	118.95 (12)	P1—Pd1—Cl1	85.63 (4)
O3—P1—Pd1	114.05 (12)	P2—Pd1—Cl1	176.07 (4)
O4—P2—O5	94.95 (16)	P1—Pd1—Cl2	176.26 (4)
O4—P2—O6	105.28 (16)	P2—Pd1—Cl2	85.46 (4)
O5—P2—O6	107.18 (17)	Cl1—Pd1—Cl2	90.74 (4)

Data collection: *EXPOSE* (Stoe, 1997); cell refinement: *CELL* (Stoe, 1997); data reduction: *INTEGRATE* (Stoe, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

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