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## Key indicators

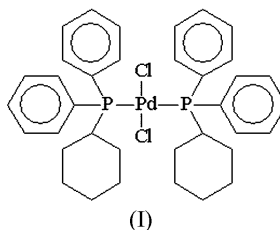
Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$   
 $R$  factor = 0.042  
 $wR$  factor = 0.105  
Data-to-parameter ratio = 22.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*trans*-Dichlorobis(cyclohexyldiphenylphosphine)-  
palladium(II)

As part of a systematic investigation for a number of Pd<sup>II</sup> complexes in order to find correlations between molecular structure and chemical behaviour, crystals of the title compound, *trans*-[PdCl<sub>2</sub>(PPh<sub>2</sub>Cy)<sub>2</sub>] or [PdCl<sub>2</sub>(C<sub>18</sub>H<sub>21</sub>P)<sub>2</sub>], were prepared. The Pd atom is located on an inversion center. Selected geometrical parameters are: Pd–P 2.3256 (10) and Pd–Cl 2.3007 (11) Å, and P–Pd–Cl 91.38 (4)°. The effective and Tolman cone angles for the PPh<sub>2</sub>Cy ligand were determined as 151.0 and 154.6°, respectively.

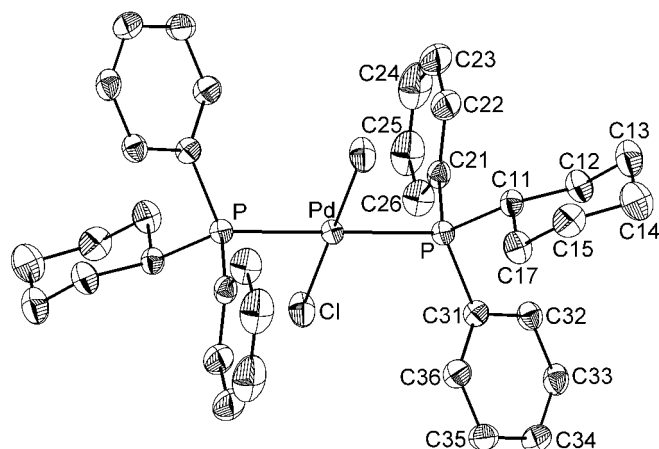
Received 22 November 2002  
Accepted 11 December 2002  
Online 24 December 2002

## Comment

The title compound, *trans*-[PdCl<sub>2</sub>(PPh<sub>2</sub>Cy)<sub>2</sub>], (I), crystallizes in the monoclinic space group  $P2_1/n$ , with the Pd atom on an inversion centre and each pair of equivalent ligands in a mutually *trans* orientation. The geometry is, therefore, square planar and all the angles in the coordination polyhedron are very close to the ideal value of 90°, with P–Pd–Cl = 91.38 (4)° and P–Pd–Cl<sup>i</sup> = 88.62 (4)° [see Table 1; symmetry code: (i)  $-x, -y, -z$ ]. The P–Pd–P<sup>i</sup> and Cl–Pd–Cl<sup>i</sup> angles are 180°, as required by the crystallographic symmetry. The bond distance P–C11 of 1.837 (3) Å (cyclohexyl moiety) is somewhat longer than the bond distances for the phenyl moieties, where P–C21 = 1.817 (3) Å and P–C31 = 1.819 (3) Å. The C–C bond distances in the phenyl rings agree well with the expected value. The average C–C bond distances for the C21–C26 and C31–C36 phenyl moieties are 1.395 (5) and 1.378 (6) Å, respectively. The average C–C bond distance for the cyclohexyl moiety (C11–C16) is 1.494 (5) Å. The C–C–C angles in the phenyl rings ( $sp^2$



hybridization) are all normal, with an average value of 119.9 (5)°, while the average ring angle for the cyclohexyl (Cy) ring ( $sp^3$  hybridization) is 113.3 (5)°. The cyclohexyl ring (ring 1) has a normal chair conformation, with torsion angles ranging from 47.1 (5) to 51.9 (5)°. The effective ( $\theta_E$ ; Otto, 2001) and Tolman cone angles ( $\theta_T$ ; Tolman, 1977) for the PPh<sub>2</sub>Cy ligand were determined as 151.0 and 154.6°, respectively, using the actual Pd–P bond length and a distance of 2.28 Å according to definition. A van der Waals radius of 1.2 Å for hydrogen and C–H bond distances of 0.97 Å for CH<sub>2</sub> and 0.93 Å for CH were used.



**Figure 1**

The structure of (I), showing the atom-numbering scheme and displacement ellipsoids at the 30% probability level. The H atoms have been omitted for clarity.

In Table 2, the title compound is compared with other closely related Pd<sup>II</sup> complexes from the literature containing two chloro and two tertiary phosphine ligands in a *trans* geometry. Compound (I), having a Pd–Cl bond length of 2.3007 (11) Å and a Pd–P bond length of 2.3256 (10) Å, fits well into the typical range for complexes of this kind.

## Experimental

Dichloro(1,5-cyclooctadiene)palladium(II), [PdCl<sub>2</sub>(COD)], was prepared according to the literature procedure of Drew & Doyle (1990). Diphenylcyclohexylphosphine (19.7 mg, 0.076 mmol) was added to a solution of [PdCl<sub>2</sub>(COD)] (10 mg, 0.035 mmol) in dichloromethane (10 ml), and slow evaporation of the solvent gave yellow crystals of *trans*-[PdCl<sub>2</sub>(PPh<sub>2</sub>Cy)<sub>2</sub>] suitable for X-ray analysis.

### Crystal data

[PdCl<sub>2</sub>(C<sub>18</sub>H<sub>21</sub>P)<sub>2</sub>]  
*M<sub>r</sub>* = 713.98  
 Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 9.797 (5) Å  
*b* = 12.552 (5) Å  
*c* = 14.087 (5) Å  
 $\beta$  = 94.357 (5)°  
*V* = 1727.3 (13) Å<sup>3</sup>  
*Z* = 2

*D<sub>x</sub>* = 1.373 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 204 reflections  
 $\theta$  = 3–23°  
 $\mu$  = 0.81 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Cuboid, yellow  
 0.20 × 0.19 × 0.10 mm

### Data collection

Bruker SMART 1000 CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1998)  
*T<sub>min</sub>* = 0.86, *T<sub>max</sub>* = 0.92  
 11 930 measured reflections

4236 independent reflections  
 2604 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.050  
 $\theta_{max}$  = 28.3°  
*h* = –10 → 13  
*k* = –15 → 16  
*l* = –15 → 18

### Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.042  
*wR* (*F*<sup>2</sup>) = 0.106  
*S* = 0.95  
 4236 reflections  
 187 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.0819P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.007$   
 $\Delta\rho_{max} = 0.65 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.74 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Pd–Cl	2.3007 (11)	P–C21	1.817 (3)
Pd–P	2.3256 (10)	P–C11	1.837 (3)
P–C31	1.819 (3)		
Cl–Pd–P	91.38 (4)	C21–P–Pd	103.79 (11)
C31–P–Pd	117.68 (11)	C11–P–Pd	117.12 (11)

**Table 2**

Comparative geometrical parameters for selected *trans*-[PdCl<sub>2</sub>(*L*)<sub>2</sub>] (*L* = tertiary phosphine ligand) complexes.

<i>L</i>	Pd– <i>L</i> (Å)	Pd–Cl (Å)	Notes
PPh <sub>3</sub>	2.337 (1)	2.290 (1)	i
PPh <sub>3</sub>	2.345 (1)	2.296 (1)	ii
	2.353 (1)	2.281 (1)	
PCy <sub>3</sub>	2.3628 (9)	2.3012 (9)	iii
PPh( <sup><i>i</i></sup> Bu) <sub>2</sub>	2.398 (2)	2.301 (2)	iv
PPh <sub>2</sub> Cy	2.3257 (9)	2.2995 (9)	v
PPh <sub>2</sub> ( <i>p</i> - <sup><i>t</i></sup> BuNO)Ph)	2.3298 (6)	2.2865 (7)	vi
pPhqH <sub>2</sub> <sup>a</sup>	2.343 (3)	2.302 (3)	vii
pPhqMe <sub>2</sub> <sup>b</sup>	2.337 (1)	2.307 (1)	vii
PPh <sub>2</sub> CHCO <sub>2</sub> H)	2.326 (1)	2.305 (1)	viii
PPh <sub>2</sub> (NC <sub>5</sub> H <sub>10</sub> )	2.324 (2)	2.289 (2)	ix

† Notes: Cy is cyclohexyl, (a) pPhqH<sub>2</sub> = *p*-hydroquinonylphosphine, (b) pPhqMe<sub>2</sub> = *p*-hydroquinonyldimethyletherphosphine; (i) Ferguson *et al.* (1982); (ii) Kitano *et al.* (1983); (iii) Grushin *et al.* (1994); (iv) DiMeglio *et al.* (1990); (v) this work; (vi) Leznoff *et al.* (1999); (vii) Sembiring *et al.* (1995); (viii) Edwards *et al.* (1998); (ix) Burrow *et al.* (1994).

H atoms were treated as riding, with C–H = 0.93, 0.97 and 0.98 Å for those on phenyl, secondary and tertiary C atoms, respectively.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: DIAMOND (Brandenburg & Brendt, 2001); software used to prepare material for publication: WinGX (Farrugia, 1999).

Financial assistance from the Rand Afrikaans University is gratefully acknowledged.

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