Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chloro[*N*-(diphenylphosphino)pyridin-2-amine-κ^2N^1,P](diphenylphosphoryl)palladium(II)

Peng Li, Qing-Shan Li,* Feng-Bo Xu, Hai-Bin Song and Zheng-Zhi Zhang

State Key Laboratory and Institute of Elemento-Organic Chemistry, Nankai University, Tianjin, Weijin road No 94,Tianjin, People's Republic of China

Correspondence e-mail: nkpengli@mail.nankai.edu.cn

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.014 Å
R factor = 0.057
wR factor = 0.123
Data-to-parameter ratio = 17.5

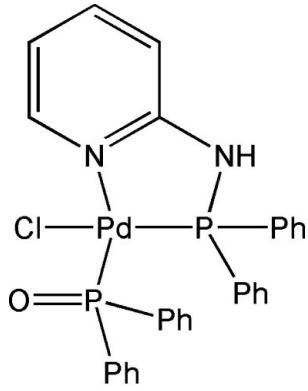
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 30 June 2006
Accepted 5 July 2006

In the title compound, $[Pd(C_{12}H_{10}OP)Cl(C_{17}H_{15}N_2P)]$, the Pd^{II} atom adopts a square-planar coordination geometry.

Comment

Phosphine ligands and their complexes play a very important role in coordination chemistry (Zhang & Cheng, 1996). Their synthesis and reactivity has attracted considerable interest owing to their novel structural and reactive features, and their potential application as catalysts (David *et al.*, 1997). Previously, we have reported an unexpected Pt^{II} complex with a rearranged phosphine ligand, *N*-(diphenylphosphino)-*N*-[(diphenylphosphoryl)methyl]pyridin-2-amine (Li *et al.*, 2006). Treatment of the above ligand with $Pd(cod)Cl_2$ (where cod is 1,5-cyclooctadiene) in dichloromethane yielded the unexpected title complex, (I), in which the phosphine ligand was cleaved and oxidized into two parts, which are coordinated to the Pd atom.



(I)

As shown in Fig.1, the Pd^{II} atom is coordinated by one N and one P atom from an *N*-(diphenylphosphino)pyridin-2-amine ligand, one P atom from a diphenylphosphoryl ligand and a chloride anion, in a square-planar coordination. The Pd—P bond *trans* to N is longer than that *trans* to Cl by *ca* 0.056 Å (Table 1). The dihedral angle between the five-membered chelate ring and the pyridine ring is 6.4 (1)°.

Experimental

The *N*-(diphenylphosphino)-*N*-[(diphenylphosphoryl)methyl]pyridin-2-amine ligand was prepared according to the literature method of Li *et al.* (2006). Complex (I) was obtained from the treatment of the above ligand (0.142 g, 0.25 mmol) with $Pd(cod)Cl_2$ (0.072 g, 0.25 mmol) in dichloromethane (yield 0.102 g, 66%). Single crystals

of (I) were obtained by slow evaporation of a dichloromethane solution.

Crystal data

$[Pd(C_{12}H_{10}OP)Cl(C_{17}H_{15}N_2P)]$	$Z = 8$
$M_r = 621.30$	$D_x = 1.520$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo $K\alpha$ radiation
$a = 13.226$ (2) Å	$\mu = 0.93$ mm^{-1}
$b = 13.594$ (2) Å	$T = 294$ (2) K
$c = 30.205$ (5) Å	Block, pale yellow
$V = 5430.7$ (15) Å^3	0.22 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer	29378 measured reflections
φ and ω scans	5756 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	3130 reflections with $I > 2\sigma(I)$
$T_{min} = 0.822$, $T_{max} = 0.866$	$R_{int} = 0.099$
	$\theta_{max} = 26.8°$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.057$	$w = 1/[\sigma^2(F_o^2) + 29.0746P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.123$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.12$	$\Delta\rho_{max} = 0.81$ e Å^{-3}
5756 reflections	$\Delta\rho_{min} = -0.94$ e Å^{-3}
329 parameters	

Table 1
Selected geometric parameters (Å, °).

Pd1—N1	2.162 (5)	Pd1—P2	2.2739 (18)
Pd1—P1	2.2178 (19)	Pd1—Cl1	2.3609 (19)
N1—Pd1—P1	82.61 (15)	N1—Pd1—Cl1	92.93 (16)
N1—Pd1—P2	174.06 (16)	P1—Pd1—Cl1	173.45 (7)
P1—Pd1—P2	91.48 (7)	P2—Pd1—Cl1	93.01 (7)

The N-bound H atom was located in a difference map and refined freely [N—H = 0.85 (6) Å]. The C-bound H atoms were positioned geometrically, with C—H = 0.93 Å and were constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

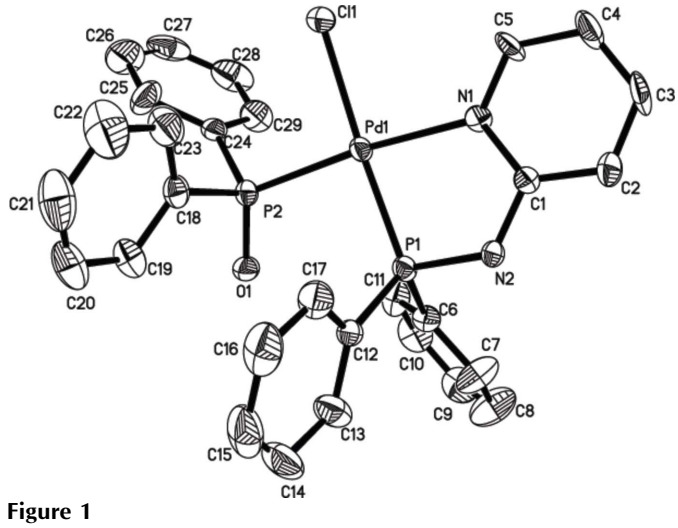


Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation of China (grant No. 20472036)

References

Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
David *et al.* (1997). *J. Am. Chem. Soc.* **119**, 7778–7790.
Li, P., Li, Q.-S., Xu, F.-B., Song, H.-B. & Zhang, Z.-Z. (2006). *Acta Cryst.* E**62**, m1575–m1576.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, Z. Z. & Cheng, H. (1996). *Coord. chem. Rev.* **147**, 1–39.