Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

trans-Dichlorodipyridinepalladium(II)

Chuang-Yi Liao and Hon Man Lee*

National Changhua University of Education, Department of Chemistry, Changhua, Taiwan 50058

Correspondence e-mail: leehm@cc.ncue.edu.tw

Received 23 February 2006
Accepted 24 February 2006

In the structure of the title compound, $[PdCl_2(C_5H_5N)_2]$, determined at 150 K, the Pd atom is located on an inversion centre. The structure is a polymorph of a previously reported structure [Viossat *et al.* (1993). *Acta Cryst.* C**49**, 84–85].

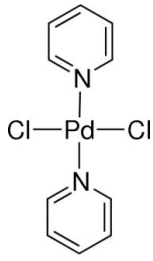
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
R factor = 0.024
wR factor = 0.065
Data-to-parameter ratio = 19.3

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

Comment

Our group is interested in the preparation of palladium complexes of *N*-heterocyclic carbene (NHC) ligands (Lee *et al.*, 2004). A general synthetic method is *via* the *in situ* deprotonation of the corresponding imidazolium salt to generate the NHC ligand, which is then trapped by a suitable palladium precursor. In the course of preparing a palladium dichloride complex supported by a monodentate NHC ligand, we reacted the corresponding imidazolium salt, palladium dichloride, and pyridine as both solvent and base. Under unoptimized conditions, the title compound, (I), was the sole product.



(I)

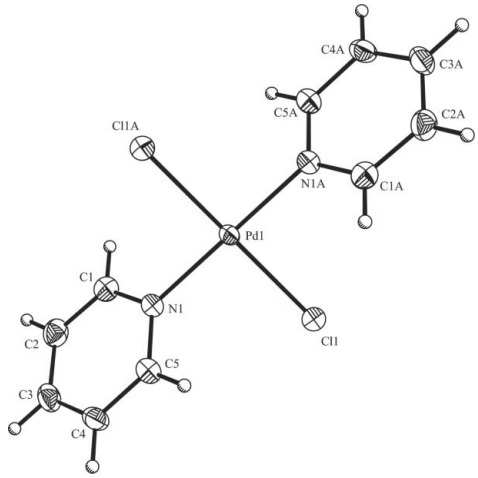


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids for non-H atoms. [Symmetry code: (A) $1-x, 1-y, -z$.]

We present here the structure of (I) (Fig. 1). It crystallizes in the centrosymmetric space group $P\overline{1}$ with the palladium centre situated at a centre of inversion. The structure is a polymorph of a previously determined structure (Viossat *et al.*, 1993). The marked difference between these two structures is the coplanarity of the two pyridine rings in (I); in the other polymorph, the two pyridine planes make an angle of 20.0 (5)°.

Experimental

The title compound is commerically available. Crystals were grown by slow diffusion of diethyl ether into a dimethylformamide solution of the compound.

Crystal data

$[PdCl_2(C_5H_5N)_2]$	$Z = 1$
$M_r = 335.50$	$D_x = 1.955$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 5.4624$ (3) Å	Cell parameters from 2287 reflections
$b = 6.9863$ (4) Å	$\theta = 3.0$–$27.8°$
$c = 7.5977$ (5) Å	$\mu = 2.06$ mm^{-1}
$\alpha = 80.852$ (4)°	$T = 150$ (2) K
$\beta = 84.578$ (4)°	Block, orange
$\gamma = 89.163$ (4)°	0.12 × 0.11 × 0.07 mm
$V = 284.97$ (3) Å^3	

Data collection

Bruker SMART APEX-II diffractometer	1352 independent reflections
ω scans	1329 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$R_{int} = 0.013$
$T_{min} = 0.790$, $T_{max} = 0.869$	$\theta_{max} = 27.9°$
3106 measured reflections	$h = -7 \rightarrow 7$
	$k = -9 \rightarrow 9$
	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0193P)^2 + 0.8582P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.024$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.065$	$\Delta\rho_{max} = 1.08$ e Å^{-3}
$S = 1.14$	$\Delta\rho_{min} = -0.52$ e Å^{-3}
1352 reflections	
70 parameters	
H-atom parameters constrained	

All H atoms were positioned geometrically (C—H = 0.95 Å) and refined with a riding model, with $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms and $1.2U_{eq}(C)$ for all other H atoms. The highest peakin the electron-density map is 1.08 Å from atom H4.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the National Science Council of Taiwan for financial support.

References

Bruker (2004). *APEX2*. Version 1.0-22. Bruker AXS Inc., Madison, Wisconsin, USA.
Lee, H. M., Lu, C. Y., Chen, C. Y., Chen, W. L., Lin, H. C., Chiu, P. L. & Cheng, P. Y. (2004). *Tetrahedron*, **60**, 5807–5825.
Sheldrick, G. M. (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2003). *SADABS*. Verion 2.10. University of Göttingen, Germany.
Viossat, B., Dung, N.-H. & Robert, F. (1993). *Acta Cryst.* C**49**, 84–85.