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Dichlorobis(1-methyl-1,4,5,6-tetrahydropyrimidine)palladium(II)

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Key indicators

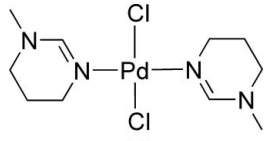
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.022
wR factor = 0.056
Data-to-parameter ratio = 21.3

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

In the structure of the title compound, $[PdCl_2(C_5H_{10}N_2)_2]$, at 150 K, the Pd atom is situated on a centre of inversion. The geometry of the complex is similar to that of *trans*-bis(1-benzylimidazole)dichloropalladium(II).

Comment

We are interested in the preparation of new *N*-heterocyclic carbene (NHC) ligands and their palladium complexes (Chiu *et al.*, 2005). In this context, we commenced a project to prepare new NHC ligand precursors based on 1-methyl-1,4,5,6-tetrahydropyrimidine. Unexpectedly, under unoptimized reaction conditions, we obtained the title compound, (I), as a minor impurity.



(I)

In the structure of (I) at 150 K, the Pd atom is situated on a centre of inversion (Fig. 1). The geometry of the complex is similar to that of *trans*-bis(1-benzylimidazole)dichloropalladium(II), (II), reported by us recently (Chen & Lee, 2006). In (I), the organic ligands twist away from the square coordination plane with a C1—N1—Pd1—Cl1 torsion angle of 43.47 (14)°. In (II), twisting of the imidazole group of the organic ligand results in a corresponding torsion angle of 31.93 (12)°.

Experimental

The crystal used for this study was obtained as a minor impurity from an unpublished procedure of ours. Alternatively, the compound can be independently prepared by heating a mixture of palladium dichloride (0.150 g, 0.845 mmol) and 1-methyl-1,4,5,6-tetrahydropyrimidine (0.166 g, 1.69 mmol) in DMF (10 ml). After cooling, removal of the solvent under vacuum affords an orange solid (yield 0.221 g, 70%). Crystals suitable for structural analysis can be obtained by vapour diffusion of diethyl ether into an acetonitrile solution of (I).

Crystal data

$[PdCl_2(C_5H_{10}N_2)_2]$
M_r = 373.60
Monoclinic, $P2_1/n$
a = 8.0324 (2) Å
b = 8.3664 (2) Å
c = 10.8658 (3) Å
β = 104.008 (2)°
V = 708.49 (3) Å^3
Z = 2
D_x = 1.751 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.67 mm^{-1}
T = 150 (2) K
Block, orange
0.16 × 0.12 × 0.09 mm

Data collection

Bruker SMART APEXII CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.776, T_{max} = 0.864
5267 measured reflections
1679 independent reflections
1432 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.9°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.057
S = 1.04
1679 reflections
79 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

All H atoms were positioned geometrically (C—H = 0.95–0.99 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.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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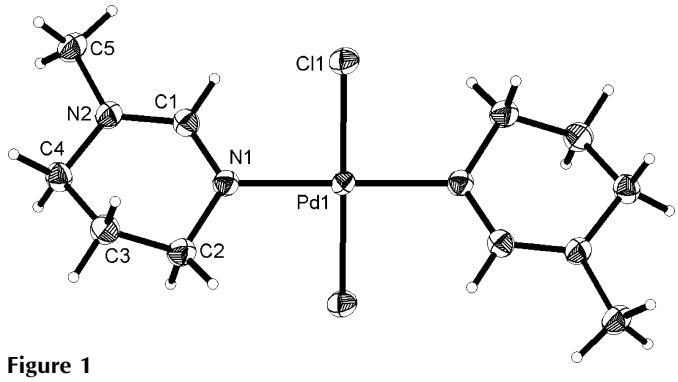

Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 50% probability level for non-H atoms. H atoms are of arbitrary size. Unlabelled atoms are related to labelled atoms by the symmetry operation $(-x, 1 - y, 1 - z)$.

References

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