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trans-Bis(1-benzylimidazole)dichloropalladium(II)

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The structure of the title compound, $[PdCl_2(C_{10}H_{10}N_2)_2]$, has the palladium center situated on a center of inversion. The imidazole group is twisted from the square coordination plane with a C—N—Pd—Cl torsion angle of 31.93 (12)°; this is different from the angle reported in closely related structures.

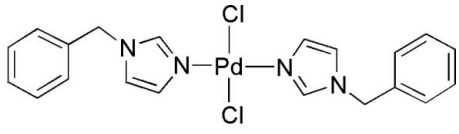
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.018
wR factor = 0.048
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 mulitdentate NHC ligand, we reacted the corresponding imidazolium salt and palladium dichloride. An unsuccessful attempt resulted in the decomposition product *trans*-bis(1-benzylimidzole)dichloropalladium(II), (I), which can be independently prepared by the reaction between 1-benzylimidazole and palladium(II) dichloride in dimethyl sulfoxide (DMSO).



(I)

Here, we present the structure of (I) (Fig. 1). It crystallizes in the monoclinic space group $P2_1/n$ with the palladium center situated at a center of inversion. The imidazole unit is twisted away from the square coordination plane, with a C2—N2—

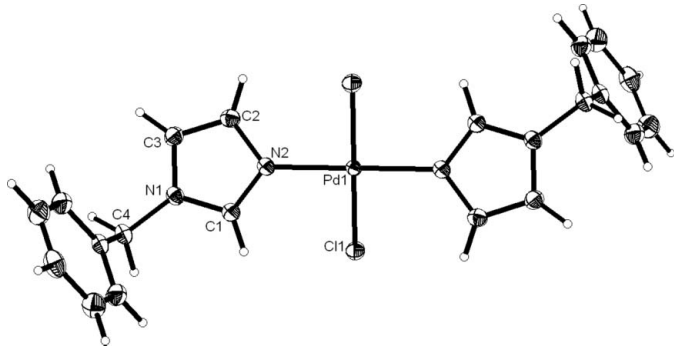


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids for non-H atoms. H atoms are of arbitrary size. Unlabeled atoms are related to labeled atoms by $(1-x, -y, -z)$.

Pd1—Cl1 torsion angle of 31.93 (12)°. The corresponding angles in a closely related structure with an *N*-*n*-propyl substituent on the imidazole ligand are, however, 19.0 (3) and 23.0 (3)° (Ianelli *et al.*, 1985), whereas that in another complex with an *N*-vinyl substituent is 47.6 (1)° (Kurdziel & Glowiak, 2002).

Experimental

A mixture of 1-benzylimidazole (0.221 g, 1.40 mmol) and palladium(II) dichloride (0.124 g, 0.700 mmol) was heated at 363 K for 2 d in DMSO (10 ml). After cooling, the solvent was removed completely under vacuum to afford a yellow solid (yield 0.283 g, 82%). Crystals suitable for structural analysis were obtained by vapor diffusion of diethyl ether into a dimethylformamide solution containing the solid.

Crystal data

$[PdCl_2(C_{10}H_{10}ClN_2)_2]$
M_r = 493.70
Monoclinic, $P2_1/n$
a = 6.7632 (1) Å
b = 20.6542 (4) Å
c = 7.5512 (1) Å
β = 112.749 (2)°
V = 972.76 (3) Å^3
Z = 2
D_x = 1.686 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 150 (2) K
Prism, yellow
0.25 × 0.20 × 0.17 mm

Data collection

Bruker SMART APEXII diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.747, T_{max} = 0.817
9632 measured reflections
2393 independent reflections
2170 reflections with $I > 2\sigma$
R_{int} = 0.018
θ_{max} = 28.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.048
S = 1.06
2393 reflections
124 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0249P)^2 + 0.4092P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

All H atoms were positioned geometrically and refined with a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ and C—H = 0.95–0.99 Å.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; 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*.

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