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Dichlorobis(*N*-methylaniline)palladium(II)

E Yang,[a]* Yao Kang[b] and Gu-Yong Chen[a]

[a]College of Chemistry & Materials Science, Fujian Normal University, Fuzhou, Fujian 350007, People's Republic of China, and [b]The State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, People's Republic of China

Correspondence e-mail: yangeli66@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.020 Å
R factor = 0.074
wR factor = 0.193
Data-to-parameter ratio = 15.6

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

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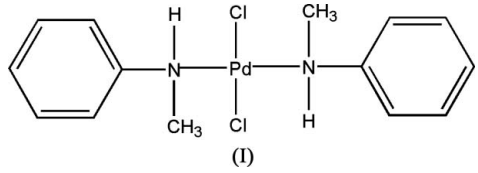
The title complex, $[PdCl_2(C_7H_9N)_2]$, has crystallographic inversion symmetry. It forms a layered structure through N—H···Cl hydrogen bonds. The Pd^{II} ion is in a square-planar coordination.

Comment

Although many studies have been reported for $C_6H_5NH_2$ compounds (Chen *et al.*, 2002) and related complexes (Newkome *et al.*, 1982; Navarro-Ranninger *et al.*, 1983*a*,*b*; Bell *et al.*, 1966), no complex has been reported which contains the $C_6H_5NH(CH_3)$ ligand. We report here the first $C_6H_5NH(CH_3)$ complex, *viz*. $[PdCl_2(C_7H_9N)_2]$, (I).



(I)

The X-ray crystallographic analysis of (I) reveals that the Pd atom, on an inversion centre, is coordinated in a square-planar fashion by the Cl and N atoms (Fig. 1). The Pd—N and Pd—Cl bond distances are comparable to those in $[PdCl_2(C_6H_5NH_2)_2]$ (Chen *et al.*, 2002). There are pairwise N—H···Cl hydrogen bonds that link the complexes together, forming layers (Fig. 2). These hydrogen bonds are slightly shorter than those in $[PdCl_2(C_6H_5NH_2)_2]$ complexes (Chen *et al.*, 2002).

Experimental

A mixture of $C_6H_5NH(CH_3)$ (10 ml), $PdCl_2$ (0.17 g) and CH_3CN (20 ml) was stirred at about 353 K for 2 h and then filtered. The filtrate was kept at room temperature for several days to give yellow crystals of the title complex, (I).

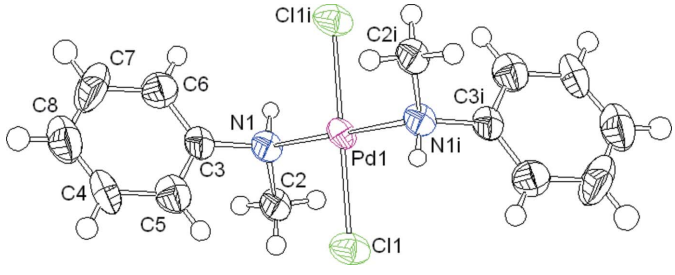


Figure 1
The structure of (I), showing displacement ellipsoids at the 50% probability level. H atoms are shown as small spheres of arbitrary radii. [symmetry code: (i) $1-x, -y, 1-z$].

Crystal data

$[PdCl_2(C_7H_9N)_2]$
M_r = 391.62
Monoclinic, $P2_1/n$
a = 6.1411 (11) Å
b = 15.501 (3) Å
c = 8.5024 (17) Å
β = 103.685 (3)°
V = 786.4 (3) Å^3
Z = 2
D_x = 1.654 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.51 mm^{-1}
T = 293 (2) K
Prism, yellow
0.35 × 0.22 × 0.10 mm

Data collection

Bruker SMART 1K diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.678, T_{max} = 0.860
2765 measured reflections
1373 independent reflections
888 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.193
S = 1.08
1373 reflections
88 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0909P)^2 + 3.5006P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.38 e Å^{-3}
$\Delta\rho_{min}$ = −1.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pd1—N1	2.070 (8)	Pd1—Cl1	2.302 (3)
N1—Pd1—Cl1	94.2 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl1^{i}	0.91	2.49	3.302 (10)	149

Symmetry code: (i) $x-1, y, z$.

All H atoms were placed at calculated positions, and refined with isotropic displacement parameters, using a riding model [C—H = 0.93 or 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C); N—H = 0.91 Å and U_{iso}(H) = 1.2U_{eq}(N)]. In the final difference map, the deepest hole is 1.03 Å from atom Pd1 and the highest peak is 0.99 Å from Pd1.

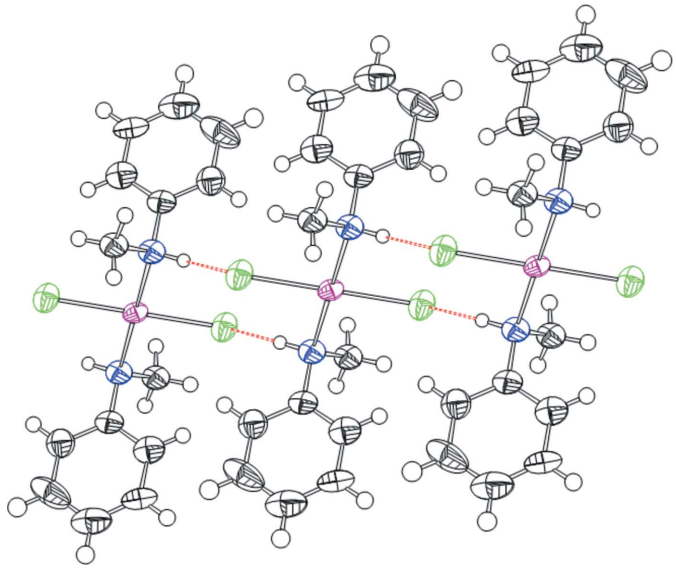


Figure 2
View of the extensive hydrogen bonding (dashed lines) between complexes.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994)); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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