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cis-(2-Amino-1,1-dimethylethylamine)dichloropalladium(II) ethanol hemisolvate

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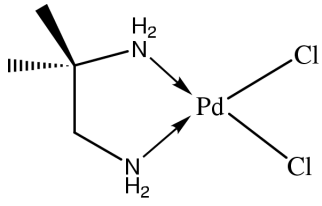
Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
Disorder in solvent or counterion
R factor = 0.026
wR factor = 0.058
Data-to-parameter ratio = 24.3

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

The title complex, $[PdCl_2(C_4H_{12}N_2)]\cdot 0.5C_2H_6O$, (I), lies in a general position with a disordered molecule of ethanol solvate on a twofold symmetry axis. It adopts the expected square-planar geometry. The electron-donating properties of the CMe_2 group attached to one N atom are apparent in the slightly shorter corresponding Pd—N distance and slightly longer Pd—Cl bond *trans* to this vector. There is a hydrogen-bonding network involving weak N—H···Cl and stronger O—H···N and N—H···O interactions, in a chain parallel to the *c* axis.



0.5 EtOH

(I)

Experimental

The title compound was crystallized from ethanol. It is a serendipitous hydrolysis product of a Schiff base palladium(II) complex.

Crystal data

$[PdCl_2(C_4H_{12}N_2)]\cdot 0.5C_2H_6O$
M_r = 288.49
Monoclinic, *I*2/*a*
a = 16.435 (5) Å
b = 7.562 (5) Å
c = 16.527 (4) Å
β = 90.28 (2)°
V = 2053.9 (16) Å^3
Z = 8
D_x = 1.866 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3005 reflections
θ = 2–30.0°
μ = 2.27 mm^{-1}
T = 150 (2) K
Rectangular block, yellow–green
0.20 × 0.08 × 0.08 mm

Data collection

KappaCCD diffractometer
CCD rotation images, thick-slice scans
Absorption correction: multi-scan (Blessing , 1995)
T_{min} = 0.727, T_{max} = 0.834
15 940 measured reflections
2993 independent reflections
2577 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 30.0°
$h = -23 \rightarrow 23$
$k = -9 \rightarrow 10$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.058
S = 1.06
2993 reflections
123 parameters
Only H-atom U's refined
$w = 1/[\sigma^2(F_o^2) + (0.0222P)^2 + 4.1385P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

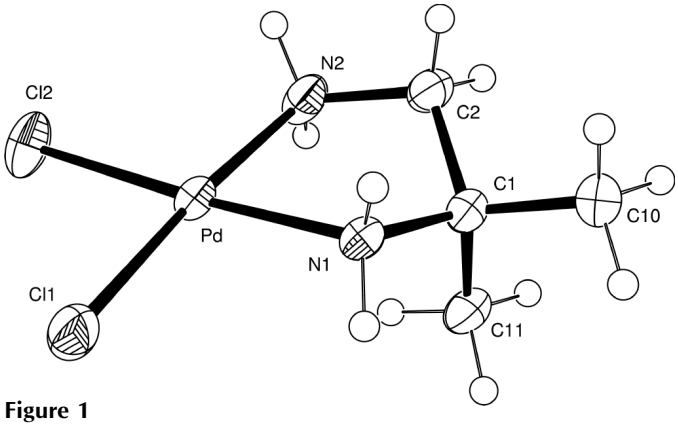


Figure 1
View of (I) (70% probability displacement ellipsoids). The disordered solvent molecule is not shown.

Table 1
Selected geometric parameters (Å, °).

Pd—N1	2.0197 (19)	N2—C2	1.488 (3)
Pd—N2	2.036 (2)	C1—C11	1.523 (4)
Pd—Cl1	2.3068 (8)	C1—C10	1.526 (3)
Pd—Cl2	2.3213 (9)	C1—C2	1.527 (3)
N1—C1	1.501 (3)		
N1—Pd—N2	83.28 (8)	N1—Pd—Cl2	175.58 (5)
N1—Pd—Cl1	90.69 (6)	N2—Pd—Cl2	92.38 (6)
N2—Pd—Cl1	173.96 (6)	Cl1—Pd—Cl2	93.66 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H12···Cl2^{i}	0.92	2.59	3.405 (3)	148
N1—H12···O100^{ii}	0.92	2.64	3.280 (9)	127
N1—H11···Cl1^{iii}	0.92	2.55	3.443 (2)	163
N2—H21···Cl2^{iv}	0.92	2.44	3.352 (3)	170
N2—H22···O100^{v}	0.92	2.07	2.873 (6)	145
N2—H22···Cl1^{i}	0.92	2.81	3.538 (3)	137
O100—H100···N2^{vi}	0.84	2.15	2.873 (6)	144

Symmetry codes: (i) $\frac{3}{2}-x,\frac{1}{2}-y,\frac{1}{2}-z$; (ii) $\frac{3}{2}-x,\frac{3}{2}-y,\frac{1}{2}-z$; (iii) $\frac{3}{2}-x,y,-z$; (iv) $\frac{3}{2}-x,-\frac{1}{2}-y,\frac{1}{2}-z$; (v) $x,y-1,z$; (vi) $x,1+y,z$.

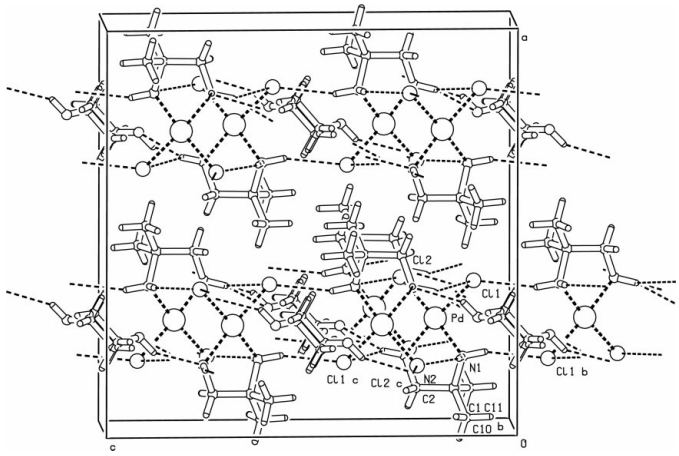


Figure 2
Unit-cell packing diagram of (I) viewed along the *b* axis.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *WinGX* (Farrugia, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines.

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