Crystal structure of bis(n-propylamine)dichloropalladium(II), $(CH_3CH_2CH_2NH_2)_2PdCl_2$

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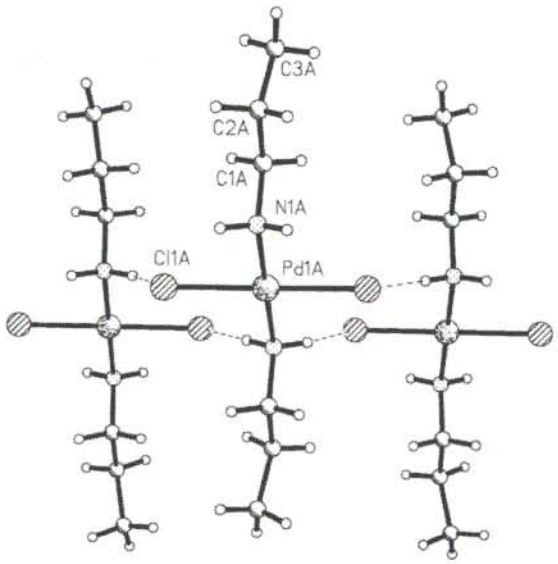

Abstract

$C_6H_{18}Cl_2N_2Pd$, monoclinic, $P12_1/c1$ (No. 14), a = 7.542(2) Å, b = 8.437(2) Å, c = 8.929(2) Å, β = 92.65(3)°, V = 567.6 Å^3, Z = 2, $R_{gt}(F)$ = 0.032, $wR(F)$ = 0.082, T = 293 K.

Source of material

The compound was obtained as a powder by reacting $PdCl_2$ with propylamine in CH_2Cl_2. Dark yellow crystals were then separated from the mother solution on standing.

Discussion

The molecular complex is centrosymmetric with the palladium atom in a quasi regular square planar configuration (the N(1)–Pd–Cl(1) angle is of 87(1)°). Relevant bond distances are: Pd–Cl 2.295(2) Å, Pd–N 2.061(8) Å, N–C 1.48(1) Å. The Pd–Cl and Pd–N distances agree well with the sum of the covalent radii (2.30 Å and 2.06 Å, respectively) [1]. The H atoms were introduced in calculated positions. Each molecule is bonded to four adjacent others through a system of Cl···H–N–H···Cl hydrogen bonding.

Table 1. Data collection and handling.

Crystal:	dark yellow prism, size 0.2 × 0.1 × 0.2 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	20.56 cm^{-1}
Diffractometer, scan mode:	Philips PW1100 (FEBO SYSTEM), 2θ
$2\theta_{max}$:	66°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1053, 1001
Criterion for F_{obs}, $N(hkl)_{gt}$:	$F_{obs} > 3\,\sigma F_{obs}$), 987
$N(param)_{refined}$:	53
Program:	SHELXL-93 [2]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1N)	4e	–0.133(1)	0.489(6)	0.6963(8)	0.08
H(2N)	4e	–0.099(1)	0.570(6)	0.7563(8)	0.08
H(11)	4e	0.356(1)	0.407(4)	0.389(1)	0.08
H(12)	4e	0.363(1)	0.593(4)	0.397(1)	0.08
H(21)	4e	0.419(2)	0.612(6)	0.146(1)	0.08
H(22)	4e	0.384(2)	0.430(6)	0.122(1)	0.08
H(31)	4e	0.689(2)	0.466(4)	0.138(2)	0.08
H(32)	4e	0.639(2)	0.375(4)	0.283(2)	0.08
H(33)	4e	0.678(2)	0.558(4)	0.290(2)	0.08

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pd(1)	2a	0	1/2	1/2	0.0132(3)	0.0184(4)	0.0106(4)	–0.001(1)	–0.0001(1)	0.0108(7)
Cl(1)	4e	0.002(1)	0.2280(3)	0.501(1)	0.083(2)	0.0410(9)	0.0427(9)	0.028(3)	0.006(1)	0.010(3)
N(1)	4e	–0.133(1)	0.489(6)	0.6963(8)	0.039(3)	0.04(1)	0.033(3)	–0.001(7)	0.004(2)	–0.014(9)
C(1)	4e	0.327(1)	0.504(4)	0.334(1)	0.043(4)	0.085(8)	0.035(4)	–0.03(1)	0.004(3)	–0.02(1)
C(2)	4e	0.431(2)	0.508(6)	0.192(1)	0.048(5)	0.10(1)	0.039(4)	–0.02(1)	0.008(3)	–0.02(1)
C(3)	4e	0.628(2)	0.474(4)	0.230(2)	0.044(4)	0.09(3)	0.058(6)	0.005(7)	0.008(4)	–0.002(8)

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References

1. Pauling, L.: The Nature of the Chemical Bond. Cornell Univ. Press, New York 1960.
2. Sheldrick, G. M.: SHELXL-93, Program for Crystal Structures Determination. University of Göttingen, Germany 1993.