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Dichlorobis[4-(methylsulfanyl)aniline-*κN*]-palladium(II)

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In the title complex, $[PdCl_2(C_7H_9NS)_2]$, the Pd atom lies on a center of inversion and is coordinated by two chloride anions and two N atoms from two benzenamine ligands to give rise to a square-planar coordination geometry for the Pd atom. A layer structure results from N—H···Cl hydrogen bonds.

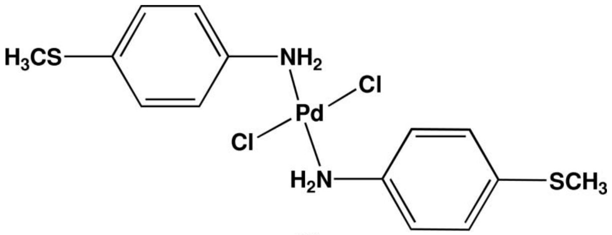
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.023
wR factor = 0.081
Data-to-parameter ratio = 17.9

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

Comment

Palladium compounds have attracted much attention as a consequence of their applications in homogeneous and heterogeneous catalysis. For instance, these are active catalysts for the carbonylation of nitroarenes, aryl halides and alkynes (Bartolo *et al.*, 2001; Gaviño *et al.*, 2001; Gallo *et al.*, 1999). We report here the synthesis and the crystal structure of (I), a palladium dichloride adduct with 4-(methylthio)aniline, as a contribution to palladium chemistry.



(I)

The Pd atom lies on a center of inversion and is coordinated by two chloride anions and two N atoms from two substituted aniline ligands in a square-planar $PdCl_2N_2$ geometry. In the crystal structure, molecules of (I) are linked *via* N—H···Cl hydrogen bonds to form a layer structure.

Experimental

The title compound was synthesized by the solvothermal reaction between 4-(methylthio)aniline and $PdCl_2$ with a molar ratio of 2:1 in acetonitrile at 373 K for 10 h. After cooling to room temperature, orange crystals suitable for X-ray analysis were obtained.

Crystal data

$[PdCl_2(C_7H_9NS)_2]$	D_x = 1.769 Mg m^{-3}
M_r = 455.72	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2975 reflections
a = 14.5222 (19) Å	θ = 2.4–28.0°
b = 7.8998 (10) Å	μ = 1.63 mm^{-1}
c = 7.6175 (10) Å	T = 298 (2) K
β = 101.751 (2)°	Prism, orange
V = 855.58 (19) Å^3	0.21 × 0.17 × 0.15 mm
Z = 2	

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.725$, $T_{\max} = 0.792$
4730 measured reflections
1758 independent reflections
1661 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\max} = 26.5°$
$h = -18 \rightarrow 12$
$k = -9 \rightarrow 9$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.081$
$S = 1.30$
1758 reflections
98 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.0486P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.59$ e Å^{-3}
$\Delta\rho_{\min} = -0.72$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pd—N1	2.054 (2)	Pd—Cl	2.3060 (6)
N1—Pd—N1$^{\rm i}$	180	N1—Pd—Cl$^{\rm i}$	90.91 (6)
N1—Pd—Cl	89.09 (6)	Cl—Pd—Cl$^{\rm i}$	180
Cl—Pd—N1—C1	95.98 (16)	Cl$^{\rm i}$—Pd—N1—C1	−84.02 (16)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$A\cdots$Cl$^{\rm ii}$	0.90	2.50	3.376 (2)	165
N1—H1$B\cdots$Cl$^{\rm iii}$	0.90	2.50	3.321 (2)	152

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

All the H atoms were placed in geometrically idealized positions (C—H = 0.93 Å for the aromatic H atoms; C—H = 0.96 Å for the methyl H atoms; N—H = 0.90 Å) and constrained to ride on their parent atoms, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(aromatic C and N) or $1.5U_{\rm eq}$(methyl C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

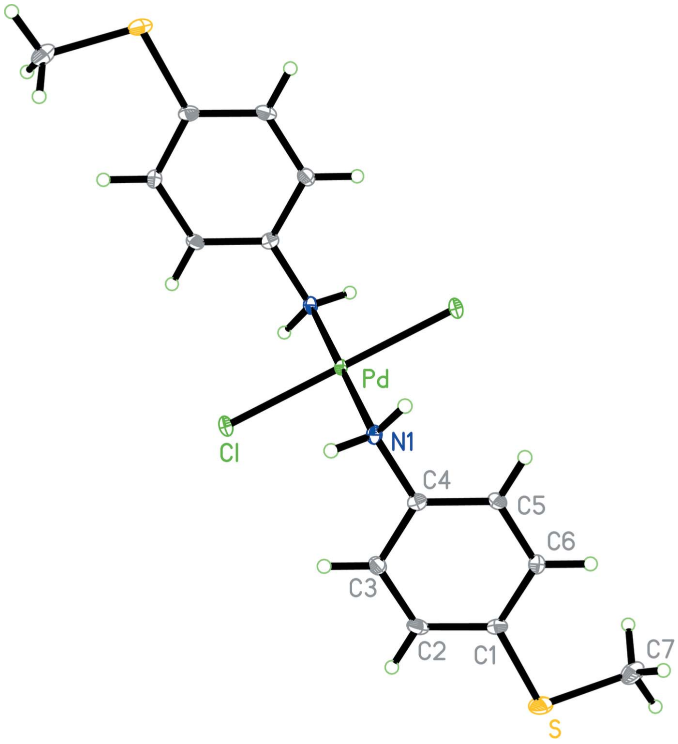


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabeled atoms are related to labeled atoms by the symmetry operation $(1-x, 1-y, 1-z)$.

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