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trans-Dichlorobis[(phenylsulfanyl)methane-*κS*]-palladium(II)

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The title compound, *trans*-[PdCl$_2$(PhSCH$_2$SPh)$_2$], crystallizes with two half-molecules in the asymmetric unit and each independent molecule lies about a crystallographic inversion center. In each molecule, one S atom of the bis(phenylsulfanyl)methane ligand is coordinated to the Pd atom while the second S atom of the same ligand is uncoordinated.

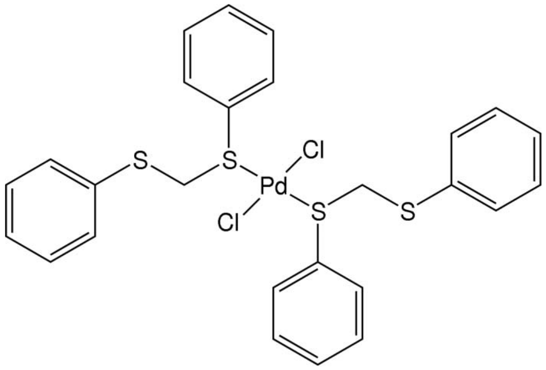
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.106
Data-to-parameter ratio = 16.6

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

Comment

Linear bifunctional ligands are usually used as building blocks for the construction of the metal-organic framework materials (MOF) (Carlucci *et al.*, 2002). Bis(phenylsulfanyl)alkanes can be used to propagate the coordination of a metal in order to form extended networks (Bu *et al.*, 2002). The title compound, (I), was prepared in the course of our studies to build coordination polymers by self-assembling linear bifunctional ligands with transition metals. The molecular structure of (I) is shown in Fig. 1. In both independent molecules, the Pd atom lies on an inversion center, thus the ligands are arranged in a *trans*-geometry. Hence, the *trans* angles are exactly 180°. The coordination is slightly disorted square-planar (Table 1). The Pd—Cl and Pd—S distances are comparable to those of the polymorph *trans*-[PdCl$_2$(PhSCH$_2$SPh)$_2$], which crystallizes in the space group $C2/c$ (Andrew *et al.*, 1994).



(I)

Experimental

The ligand bis(phenylsulfanyl)methane, PhSCH$_2$SPh, was synthesized according to the literature method of Hartley *et al.* (1979). A solution of PhSCH$_2$SPh (150 mg) in ethanol (10 ml) was reacted with Na$_2$[PdCl$_4$] (12 mg) in ethanol (5 ml). The mixture was stirred at room temperature for 2 h and evaporation of the solvent produced single crystals suitable for X-ray analysis.

Crystal data

$[PdCl_2(C_{13}H_{12}S_2)_2]$
M_r = 641.99
Triclinic, $P\overline{1}$
a = 7.7798 (1) Å
b = 11.0645 (2) Å
c = 15.4006 (3) Å
α = 85.256 (1)°
β = 82.988 (1)°
γ = 88.068 (1)°
V = 1310.88 (4) Å^3

Z = 2
D_x = 1.626 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 7199 reflections
θ = 2.9–72.7°
μ = 10.67 mm^{-1}
T = 100 (2) K
Block, colorless
0.27 × 0.11 × 0.09 mm

Data collection

Bruker SMART2000 diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min}$ = 0.176, $T_{\rm max}$ = 0.383
15821 measured reflections
4986 independent reflections

4749 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.037
$\theta_{\rm max}$ = 72.9°
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -18 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.106
S = 1.07
4986 reflections
301 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0753P)^2 + 1.085P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max}$ = 0.001
$\Delta\rho_{\rm max}$ = 1.36 e Å^{-3}
$\Delta\rho_{\rm min}$ = −1.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Pd1—Cl1^i	2.2927 (6)	Pd2—Cl2^{ii}	2.2924 (6)
Pd1—S1^i	2.3155 (6)	Pd2—S4	2.3261 (6)
Cl1^i—Pd1—Cl1	180	Cl2^{ii}—Pd2—Cl2	180
Cl1^i—Pd1—S1^i	96.21 (2)	Cl2^{ii}—Pd2—S4	84.78 (2)
Cl1—Pd1—S1^i	83.79 (2)	Cl2—Pd2—S4	95.22 (2)
S1^i—Pd1—S1	180	S4—Pd2—S4^{ii}	180

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x, -y+2, -z+1$.

H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and were included in the refinement in the riding-model approximation, with $U_{\rm iso} = 1.2U_{\rm eq}$(C). A final verification of possible voids was performed using the VOID routine of the *PLATON* program (Spek, 2003). In the final difference Fourier, the highest peak was located 1.09 Å from atom S1 and the deepest hole was 0.67 Å from Pd2.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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, 1997); software used to prepare material for publication: *UdMX* (Maris, 2004).

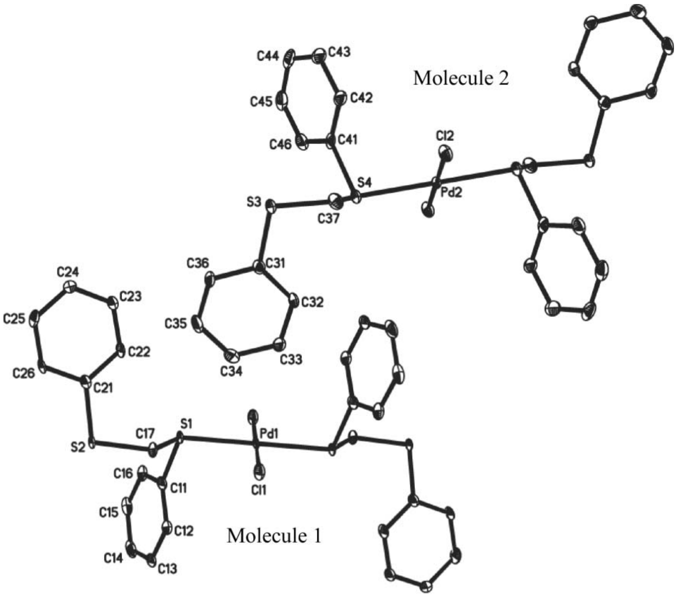


Figure 1
Views of the two independent molecules of (I), showing the atom-numbering schemes. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted. The unlabeled parts of the molecules 1 and 2 are related by the symmetry codes $(-x, 1-y, -z)$ and $(-x, 2-y, 1-z)$, respectively.

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