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[1,2-Bis(phenylsulfanyl)benzene]dichloropalladium(II)

Nobuhiro Takeda, Daisuke Shimizu, Takahiro Sasamori and Norihiro Tokitoh*

Institute for Chemical Research, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan

Correspondence e-mail: tokitoh@boc.kuicr.kyoto-u.ac.jp

In the title compound, $[PdCl_2(C_{18}H_{14}S_2)]$, the two Cl atoms and the two S atoms are in a slightly disorted square-planar arrangement around the Pd atom. The two phenyl groups are on the same side of the $PdCl_2S_2$ plane. Close contacts between the Cl and S atoms suggest weak intermolecular interactions.

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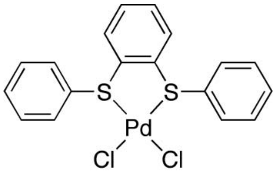
Key indicators

Single-crystal X-ray study
T = 103 K
Mean σ(C–C) = 0.003 Å
R factor = 0.017
wR factor = 0.043
Data-to-parameter ratio = 15.0

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

Comment

The synthesis and spectroscopic studies of the title compound, $[PdCl_2\{1,2\text{-}C_6H_4(SPh)_2\}]$, (I), have been performed as part of systematic studies of palladium(II) dithioether complexes (Hartley *et al.*, 1979). There is no previous report on the X-ray structural analysis of (I).



(I)

Fig. 1 shows (I) and illustrates the slightly disorted square-planar arrangement of the two Cl atoms and the two S atoms around the palladium center. The two terminal phenyl groups of the dithioether ligand are on the same side of the $PdCl_2S_2$ plane. The Pd—Cl bond lengths [Pd1—Cl1 = 2.3159 (6) and

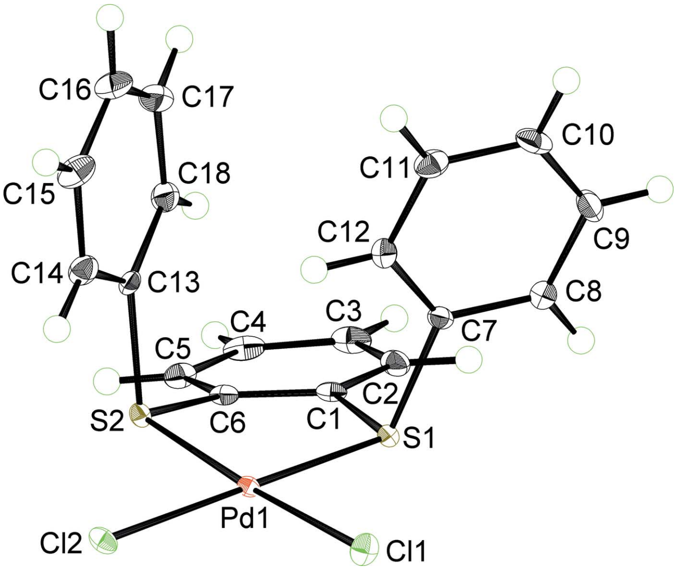


Figure 1
View of the molecule of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

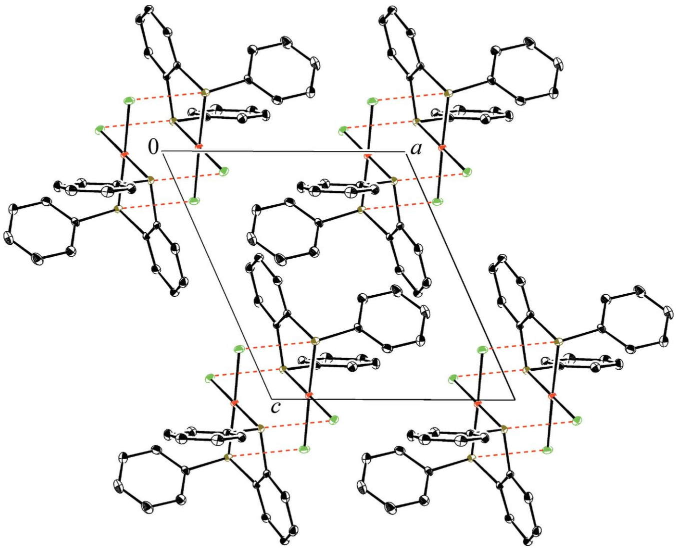


Figure 2
The molecular packing of (I), viewed along the *b* axis. H atoms have been omitted for clarity. Dashed red lines indicate the S···Cl intermolecular contacts.

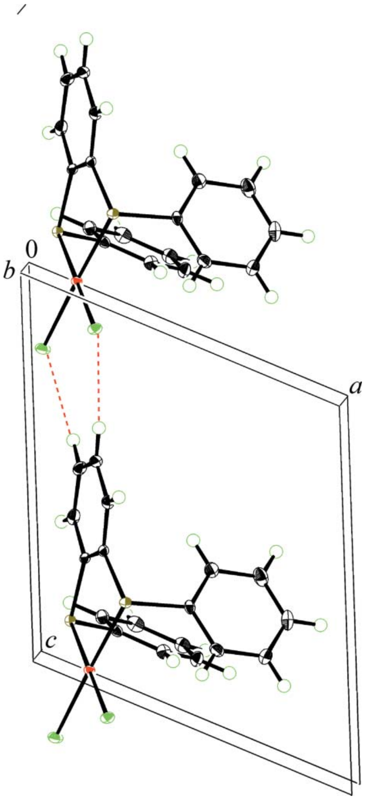


Figure 3
A section of the extended weak intermolecular C—H···Cl hydrogen-bonded (red dashed lines) chain along [001].

Pd1—Cl2 = 2.3116 (5) Å] are similar to those of reported tetracoordinate palladium(II) complexes [2.298–2.354 Å; Orpen *et al.*, 1989]. The Pd—S bond lengths [Pd1—S1 = 2.2679 (5) and Pd1—S2 = 2.2719 (6) Å] are similar to those of palladium(II) dialkylthioether complexes (2.262–2.307 Å; Orpen *et al.*, 1989).

Intermolecular Cl···S distances [S1···Cl2 = 3.3311 (9) Å and S2···Cl1 = 3.5338 (9) Å] are slightly shorter than the sum of the van der Waals radii of chlorine and sulfur (3.55 Å; Bondi, 1964). This suggests weak intermolecular interactions between the Cl and S atoms (Fig. 2). In addition, weak intermolecular C—H···Cl interactions link molecules into extended chains along [001] (see Table 2 and Fig. 3)

Experimental

1,2-Bis(phenylsulfanyl)benzene, 1,2-$C_6H_4(SPh)_2$, was prepared according to the procedure of Hartley *et al.* (1979). Sodium tetrachloropalladate (98.3 mg, 0.334 mmol) was added to an ethanol solution (20 ml) of 1,2-$C_6H_4(SPh)_2$ (100 mg, 0.340 mmol) at 343 K. Further stirring for 30 min at this temperature gave the title compound, [$PdCl_2${1,2-$C_6H_4(SPh)_2$}], (I) (155.8 mg, 0.330 mmol, 99%) [m.p. 551.4–552.4 K (decomposition)]. Suitable crystals for X-ray crystallography were obtained by slow evaporation of a chloroform/ethanol solution of (I).

Crystal data

[$PdCl_2(C_{18}H_{14}S_2)$]
M_r = 471.71
Triclinic, $P\overline{1}$
a = 9.9145 (14) Å
b = 10.214 (2) Å
c = 10.521 (2) Å
α = 76.905 (10)°
β = 63.051 (9)°
γ = 67.639 (10)°
V = 876.4 (3) $Å^3$

Z = 2
D_x = 1.787 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3041 reflections
θ = 3.0–25.5°
μ = 1.60 mm^{-1}
T = 103 (2) K
Prism, orange
0.45 × 0.30 × 0.28 mm

Data collection

Rigaku Mercury diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.534, T_{max} = 0.646
5768 measured reflections
3140 independent reflections

2982 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
θ_{max} = 25.5°
$h = -10 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -9 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.043
S = 1.09
3140 reflections
209 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0179P)^2 + 0.6226P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.34 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.47 e $Å^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0058 (6)

Table 1
Selected geometric parameters (Å, °).

Pd1—S1	2.2679 (5)	S1—C1	1.7932 (19)
Pd1—S2	2.2719 (6)	S1—Cl2^i	3.3311 (9)
Pd1—Cl2	2.3116 (5)	S2—C6	1.7774 (18)
Pd1—Cl1	2.3159 (6)	S2—C13	1.8085 (19)
S1—C7	1.7924 (18)	S2—Cl1^i	3.5338 (9)
S1—Pd1—S2	89.86 (2)	C7—S1—C1	102.47 (8)
S1—Pd1—Cl2	177.782 (16)	C7—S1—Pd1	109.26 (6)
S2—Pd1—Cl2	88.56 (2)	C1—S1—Pd1	103.51 (6)
S1—Pd1—Cl1	87.95 (2)	C6—S2—C13	100.23 (9)
S2—Pd1—Cl1	176.378 (17)	C6—S2—Pd1	102.86 (6)
Cl2—Pd1—Cl1	93.70 (2)	C13—S2—Pd1	101.01 (6)

Symmetry code: (i) $-x, -y+1, -z+2$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H2···Cl1^{ii}	0.95	2.82	3.753 (2)	169
C4—H3···Cl2^{ii}	0.95	2.66	3.513 (2)	150

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

All H atoms were treated as riding, with C—H distances of 0.95 Å and $U_{\rm iso} = 1.2U_{\rm eq}$(C).

Data collection: *CRYSTALCLEAR* (Rigaku, 2004); cell refinement: *CRYSTALCLEAR*; data reduction: *CRYSTALCLEAR*; program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*.

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