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Dichloro[8-(1,3-benzothiazol-2-ylsulfanylmethyl)-quinoline-$\kappa N,N'$]palladium(II)

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Key indicators

Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.004 Å
R factor = 0.023
wR factor = 0.059
Data-to-parameter ratio = 14.5

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

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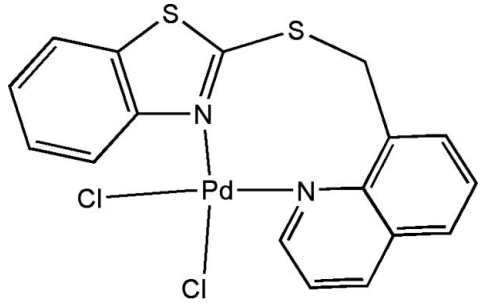
In the mononuclear title complex, $[Pd(C_{17}H_{12}N_2S_2)Cl_2]$, the 8-(2-benzothiazolylsulfanylmethyl)quinoline ligand chelates to $PdCl_2$ through its N atoms, conferring a square planar geometry on Pd. The angles around the Pd atom range from 88.04 (6) to 92.76 (3)°.

Comment

Square planar metal complexes have important applications in catalytic and bioinorganic systems (Fiallo & Garnier-Suillerot, 1986; Grundemann *et al.*, 2001; Trost *et al.*, 1995); for example, platinum(II) and palladium(II) complexes exhibit antitumour activity (Hay, 1987). The present study details the structure of a palladium dichloride adduct of a heterocyclic thioether ligand. A number of metal complexes of such ligands have been reported (Berry & Bebout, 2005; Song *et al.*, 2003; Zou *et al.*, 2004). The ligand used in this study is 8-(2-benzothiazolylsulfanylmethyl)quinoline.



(I)

The title $PdCl_2$ adduct, (I), is a mononuclear compound (Fig. 1 and Table 1), and the Pd exists in a square planar geometry formed by two Cl atoms and the two N atoms of the ligand. The quinoline and benzothiazole rings of the ligand are twisted by 96.5 (1)°; the Pd lies 0.0387 (1) Å from the square plane. The bond distances are within the ranges expected for square planar palladium (Al-Mandhary *et al.*, 2003; Buffin *et al.*, 2003; Kita *et al.*, 2002). The molecular packing in (I) is influenced by weak intermolecular C—H···Cl hydrogen bonds (Fig. 2 and Table 2).

Experimental

The ligand (30.9 mg, 0.1 mmol) in $CHCl_3$ (2 ml) was added to $PdCl_2$ (17.8 mg, 0.1 mmol) dissolved in MeCN (20 ml). The mixture was stirred for 1 min, filtered and then set aside for the solvent to evaporate. Yield 34.5 mg (70%). Analysis found: C 42.10, H 2.46, N 5.76%; calculated for $C_{17}H_{12}Cl_2N_2PdS_2$: C 42.03, H 2.49, N 5.77%.

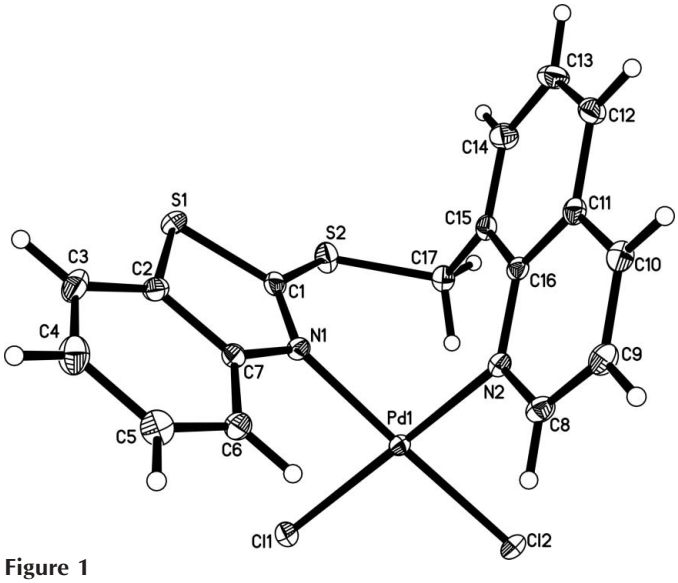


Figure 1
View of (I), shown with 30% probability displacement ellipsoids and small spheres for the H atoms.

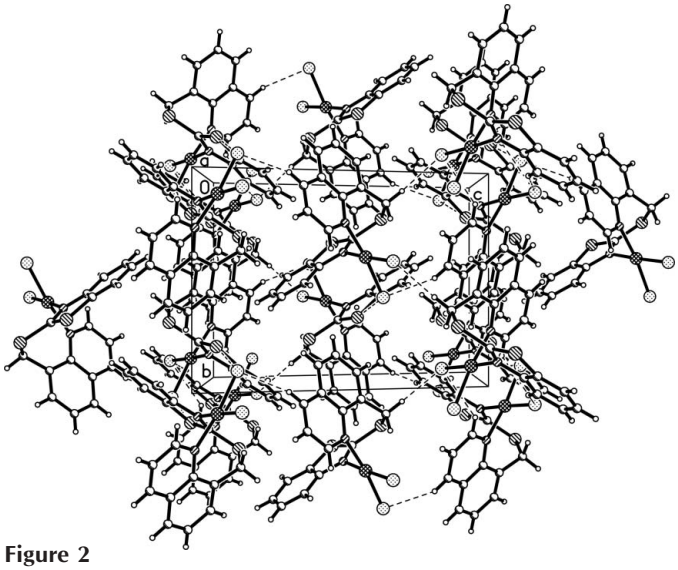


Figure 2
The molecular packing of (I) viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

Crystal data

$[Pd(C_{17}H_{12}N_2S_2)Cl_2]$	D_x = 1.867 Mg m^{-3}
M_r = 485.71	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 7287 reflections
a = 12.417 (3) Å	θ = 3.3–25.3°
b = 10.152 (3) Å	μ = 1.63 mm^{-1}
c = 14.541 (5) Å	T = 193 (2) K
β = 109.492 (5)°	Block, orange
V = 1728.0 (8) Å^3	0.46 × 0.35 × 0.23 mm
Z = 4	

Data collection

Rigaku Mercury diffractometer	3034 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.023
Absorption correction: multi-scan (Jacobson, 1998)	θ_{max} = 25.3°
T_{min} = 0.522, T_{max} = 0.706	$h = -14 \rightarrow 13$
16474 measured reflections	$k = -12 \rightarrow 12$
3157 independent reflections	$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 2.5404P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.023	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.059	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
S = 1.11	$\Delta\rho_{min}$ = −0.56 e Å^{-3}
3157 reflections	
218 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Pd1—N1	2.035 (2)	Pd1—Cl2	2.2971 (8)
Pd1—N2	2.045 (2)	Pd1—Cl1	2.3007 (8)
N1—Pd1—N2	89.52 (8)	N1—Pd1—Cl1	88.04 (6)
N1—Pd1—Cl2	177.58 (6)	N2—Pd1—Cl1	173.08 (6)
N2—Pd1—Cl2	89.94 (6)	Cl2—Pd1—Cl1	92.76 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17B···Cl2^{i}	0.99	2.75	3.667 (3)	154
C10—H10···Cl1^{ii}	0.95	2.71	3.466 (3)	137
C9—H9···Cl1^{iii}	0.95	2.94	3.658 (3)	133
C8—H8···Cl2^{iii}	0.95	2.84	3.575 (3)	135
C6—H6···Cl2^{iii}	0.95	2.73	3.571 (3)	148
C3—H3···Cl1^{iv}	0.95	2.92	3.644 (3)	134

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

H atoms were included in calculated positions and refined as riding on C, with C—H distances of 0.95 Å (aromatic H) and 0.99 Å (methylene H); U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CrystalClear* (Molecular Structure Corporation, 2000; Rigaku Corporation, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku & Rigaku/MSC, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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