Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chloro(4-methylpiperidine-1-dithiocarbamato-$\kappa^2S:S'$)-(triphenylphosphine-κP)palladium(II)

Farkhanda Shaheen,[a] Muhammad Najam-Ul-Haq,[b] Klaus Wurst,[c] Amin Badshah[a]* and Saqib Ali[a]

[a]Department of Chemistry, Quaid-I-Azam University, Islamabad 45320, Pakistan, [b]Department of Chemistry, Bahauddin Zakariya University, Multan 60800, Pakistan, and [c]Institute of General, Inorganic and Theoretical Chemistry, Innrain 52a, University of Innsbruck, A-6020 Innsbruck, Austria

Correspondence e-mail: aminbadshah@yahoo.com

Received 14 November 2005
Accepted 13 December 2005
Online 21 December 2005

Key indicators

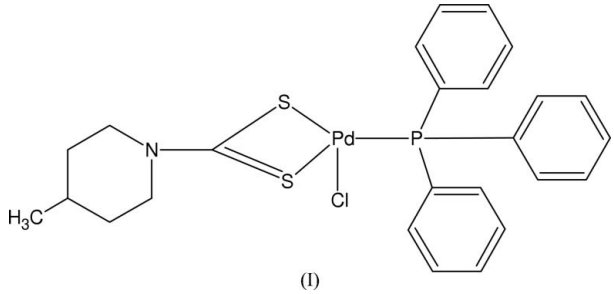
Single-crystal X-ray study
T = 233 K
Mean σ(C–C) = 0.004 Å
R factor = 0.026
wR factor = 0.061
Data-to-parameter ratio = 15.7

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

In the title compound, $[Pd(C_7H_{12}NS_2)Cl(C_{18}H_{15}P)]$, the Pd atom is four-coordinate and exhibits a slightly distorted square-planar geometry.

Comment

Palladium(II) complexes with sulfur and phosphorus donor ligands are of current interest due to their ability to sequester the metal ion (Faraglia *et al.*, 2005), their antitumor activity against leukemic cells (Mital *et al.*, 1989; Tiekink, 2002), and their use as pesticides (Fackler, 2002) and antimicrobial agents (Ronconi *et al.*, 2005), while palladium(II)–phosphine complexes are also important from a catalytic point of view (Crawforth *et al.*, 2005; Tsuji, 1995), *e.g.* $[Pd(PPh_3)_2(CN)_2]$ (Hua *et al.*, 2001), $[Pd(PPh_3)_2Cl_2]$ (Nicholas, 1987).



(I)

In the title compound, (I), the dithiocarbamate ligand acts as a bidentate chelate, coordinating to Pd *via* both S atoms. Atom S2 is *trans* to the chloro ligand and atom S1 *trans* to the triphenylphosphine ligand (Fig. 1 and Table 1). The coordination geometry about the Pd atom is distorted square planar and the deviation of the Pd1 atom from the mean plane through the ligand donor atoms is only 0.0103 (4) Å.

Experimental

4-Methylpiperidine-1-dithiocarbamic acid (Vogel, 1968) dissolved (0.2 g, 1.14 mmol) in CH_2Cl_2 (10 ml) was added to a suspension of $[PdCl_2(PPh_3)]$ (0.5 g, 1.14 mmol) (Kitano *et al.*, 1983) in CH_2Cl_2 (20 ml). The resulting solution was refluxed for 1 h. Yellow crystals were obtained on slow evaporation of the solvent at room temperature.

Crystal data

$[Pd(C_7H_{12}NS_2)Cl(C_{18}H_{15}P)]$
M_r = 578.42
Monoclinic, $P2_1/n$
a = 10.1668 (3) Å
b = 13.8325 (4) Å
c = 17.8608 (4) Å
β = 90.162 (2)°
V = 2511.79 (12) Å^3
Z = 4
D_x = 1.530 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13105 reflections
θ = 1.0–26.0°
μ = 1.09 mm^{-1}
T = 233 (2) K
Prism, yellow
0.2 × 0.12 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.025$
φ and ω scans	$\theta_{max} = 25.0^\circ$
Absorption correction: none	$h = -12 \rightarrow 12$
13105 measured reflections	$k = -16 \rightarrow 16$
4405 independent reflections	$l = -21 \rightarrow 21$
3853 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2 + 2.004P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.026$	
$wR(F^2) = 0.061$	
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.002$
4405 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
280 parameters	$\Delta\rho_{min} = -0.55$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Pd1—P1	2.3009 (7)	S1—C1	1.718 (3)
Pd1—Cl1	2.3276 (7)	S2—C1	1.735 (3)
Pd1—S1	2.3274 (7)	N1—C1	1.313 (3)
Pd1—S2	2.2977 (7)		
S2—Pd1—P1	100.32 (2)	C1—S1—Pd1	87.06 (9)
S2—Pd1—S1	75.33 (2)	C1—S2—Pd1	87.61 (9)
P1—Pd1—S1	175.24 (2)	N1—C1—S1	125.1 (2)
S2—Pd1—Cl1	166.37 (3)	N1—C1—S2	124.99 (19)
P1—Pd1—Cl1	93.29 (2)	S1—C1—S2	109.86 (14)
S1—Pd1—Cl1	91.08 (3)		

H atoms were positioned geometrically (C—H = 0.94–0.98 Å) and refined as riding, with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

We thank the Institute of Higher Education Commission for financial support of this work.

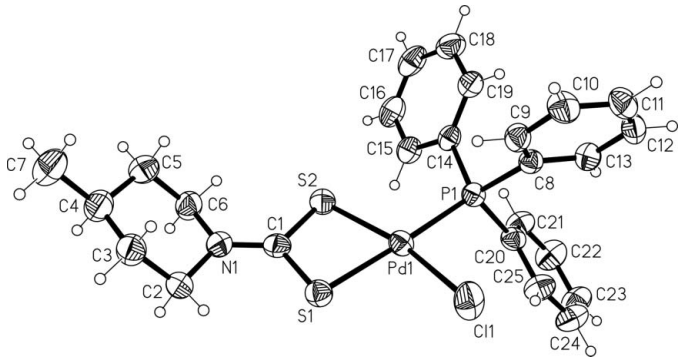


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

References

Crawforth, C. M., Burling, S., Fairlamb, I. J. S., Kapdi, A. R., Taylor, R. J. K. & Whitwood, A. C. (2005). *Tetrahedron*, **61**, 9736–9751.

Fackler, J. P. (2002). *Inorg. Chem.* **41**, 6959–6972.

Faraglia. G., Sitran, S. & Montagner, D. (2005). *Inorg. Chim. Acta*, **358**, 971–980.

Hua, R., Goto, M. & Tanaka, M. (2001). *Anal. Sci.* **17**, 469–470.

Kitano, Y., Kinoshita, Y., Nakamura, R. & Ashida, T. (1983). *Acta Cryst.* C**39**, 1015–1017.

Mital, R., Jain, N. & Srivastava, T. S. (1989). *Inorg. Chim. Acta*, **166**, 135–140.

Nicholas, P. P. (1987). *J. Org. Chem.* **52**, 5266–5272.

Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Ronconi, L., Maccato, C., Barreca, D., Saini, R., Zancato, M. & Fregona, D. (2005). *Polyhedron*, **24**, 521–531.

Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Tiekink, E. R. T. (2002). *Crit. Rev. Oncol. Hematol.* **24**, 225–248.

Tsuji, J. (1995). *Palladium Reagents and Catalysts*, pp. 125-525. New York: John Wiley and Sons.

Vogel, A. I. (1968). *A Textbook of Practical Organic Chemistry*, pp. 499–500. London: ELBS Publication.