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# (*N*,*N*-Diisopropyldithiocarbamato-*S*,*S*′)bis(triphenylphosphine-*P*)gold(**I**) butane solvate

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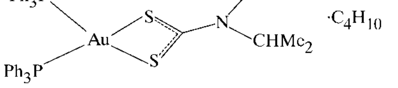
In the crystal structure of the title complex, $[Au(C_7H_{14}NS_2)(C_{18}H_{15}P)_2]\cdot C_4H_{10}$, the Au atom is in a distorted tetrahedral environment consisting of the two P atoms of the triphenylphosphine ligands and the two S atoms of the diisopropylthiocarbamate ligand. The molecular structure and packing are stablized by van der Waals interactions.

## Comment

There has been growing interest in the study of $d^{10}$ metal complexes, which exhibit rich photophysical and photochemical properties (Harvey & Gray, 1988; Vogler & Kunkely, 1988). Of particular interest is the nature of the lowest electronic excited states, which serve to develop a better understanding of the luminescent properties of $d^{10}$–$d^{10}$ systems (Yam *et al.*, 1990). Also, it has been found that gold(I) dialkyldithiocarbamates exist in discrete dimeric units which stack in the solid state to form linear gold chains (Hesse & Jennische, 1972). The number of gold(I) complexes of this type is limited in the literature. As part of our work on this type of complex, we present here the synthesis and crystal structure of the novel gold(I) complex (*N*,*N*-diisopropyldithiocarbamato-*S*,*S*′)bis(triphenylphosphine-*P*)gold(I) butane solvate, (I).



(I)

The crystal structure of (I) consists of mononuclear $[Au(PPh_3)_2\{S_2CN(^iPr)_2\}]$ units and butane molecules in a 1:1 ratio. As shown in Fig. 1, the $Au^I$ ion in (I) is four-coordinated, forming a distorted tetrahedron. The diisopropyldithiocarbamate ligand acts as a bidentate ligand coordinating through the two S atoms, forming a four-membered chelate ring. The other positions of the tetrahedron are occupied by the P atoms of two triphenylphosphine ligands.

The four-membered $AuS_2C$ ring is planar, with a maximum deviation of 0.047 (6) Å for C37. The Au1—S2 bond length [2.714 (2) Å] is longer than that of Au1—S1 [2.681 (2) Å] as the former is a coordination bond. Only a small variation in the C—S bond distance is observed. The Au—P distances are almost equal and are slightly longer than those found in $(AuSC_2H_4PEt_2)_2$ [2.27 (2) Å; Crane & Beall, 1978] and $C_{14}H_{38}Au_3Cl_3O_{12}P_6\cdot 2.5H_2O$ [2.296 (7) Å; Yam *et al.*, 1990]. The C37—N1 distance [1.350 (7) Å] has double-bond character, but is a little longer than those observed in related structures (Sharma *et al.*, 1991; Gimeno *et al.*, 1996; Jian *et al.*, 1999). The P—C and C—C bond distances are in good agreement with values reported for similar structures (Zheng *et al.*, 1997; Razak *et al.*, 2000).

The smallest angle, S1—Au1—S2 of 65.71 (5)°, is restricted by the bite angle of the ligand (Crespo *et al.*, 1997; Jones *et al.*, 1994; Gimeno *et al.*, 1994), whereas the largest angle, P1—Au1—P2 of 132.15 (5)°, is at the open side opposite the chelate ring. A possible explanation for this large value is minimization of the steric interaction between the $PPh_3$ groups. The other P—Au—S angles deviate slightly from the tetrahedral value of 109.47°.

A non-crystallographic twofold axis passes through atoms N1, C17 and Au1. The diisopropyl group is twisted by 7.5 (2)° with respect to the $AuS_2C$ group. The isopropyl groups are at anticlinal (C38, C39 and C40) and synclinal (C41, C42 and C43) orientations with respect to the N1—C38 and N1—C41 bonds, respectively. The N1—C37 bond act as an ethylene bond with S atoms and isopropyl groups on either side. The

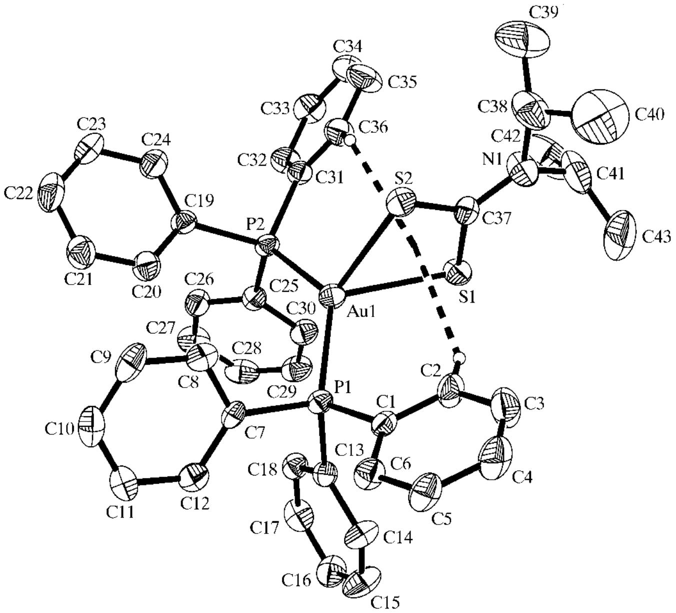


**Figure 1**
The molecular structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme; the butane solvent molecule has been omitted for clarity.

orientations of the isopropyl groups are limited by intramolecular C···S interactions. The butane solvent is not involved in any interaction as there is no potential acceptor atom.

It is quite interesting to note that the molecular structure is stabilized by intramolecular C—H···$\pi$ interactions between the aromatic H atoms of the $PPh_3$ groups and the centroid (*Cg*) of the chelate ring (atoms Au1, S1, C37 and S2) [C2···*Cg* = 3.48, H2*A*···*Cg* = 2.68 Å and C2—H2*A*···*Cg* = 145°; C36···*Cg* = 3.43, H36*A*···*Cg* = 2.72 Å and C36—H36*A*···*Cg* = 133°].

## Experimental

Sodium *N*,*N*′-diisopropyldithiocarbamate, $Na(S_2CN^iPr_2)$, dissolved in $H_2O$ was added to gold trichloride at room temperature with stirring. The brown reaction mixture was filtered and the filtrate was washed with water and dried overnight in a vacuum. The brown solid obtained was dissolved in butane. Triphenylphosphine was added at 353–363 K with stirring and the solution was refluxed for 4–5 h before cooling. Single crystals of (I) suitable for X-ray analysis were grown by slow evaporation at room temperature over a period of two weeks.

### *Crystal data*

$[Au(C_7H_{14}NS_2)(C_{18}H_{15}P)_2]\cdot C_4H_{10}$
$M_r = 955.94$
Monoclinic, $P2_1/c$
$a = 12.0927\ (2)$ Å
$b = 25.2129\ (5)$ Å
$c = 15.4999\ (3)$ Å
$\beta = 102.392\ (1)°$
$V = 4615.70\ (15)$ Å$^3$
$Z = 4$
$D_x = 1.376$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 8192 reflections
$\theta = 1.57–28.35°$
$\mu = 3.378$ mm$^{-1}$
$T = 293\ (2)$ K
Slab, colourless
0.42 × 0.28 × 0.12 mm

### *Data collection*

Siemens SMART CCD area-detector diffractometer
$\omega$ scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.331$, $T_{max} = 0.687$
31 290 measured reflections
11 360 independent reflections
5735 reflections with $I > 2\sigma(I)$
$R_{int} = 0.072$
$\theta_{max} = 28.26°$
$h = -16 \rightarrow 16$
$k = -29 \rightarrow 33$
$l = -20 \rightarrow 17$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.119$
$S = 0.988$
11 360 reflections
478 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.31$ e Å$^{-3}$
$\Delta\rho_{min} = -1.46$ e Å$^{-3}$

The butane solvent is disordered and so some atoms have a higher atomic displacement parameter ratio. All H atoms were fixed geometrically at calculated distances and allowed to ride on their parent atoms. The maximum and minimum electron densities (1.31 and −1.46 e Å$^{-3}$) were observed at distances of 1.05 and 0.89 Å, respectively, from the Au1 atom.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 1990).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1392). Services for accessing these data are described at the back of the journal.

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