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(Piperidine-1-carbodithioato-*S*,*S*′)-bis(triphenylphosphine-*P*)gold(I)

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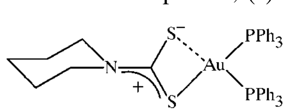
In the title compound, $[Au(C_6H_{10}NS_2)(C_{18}H_{15}P)_2]$, the Au atom is in a distorted tetrahedral environment, with the two P atoms of the triphenylphosphine ligands and the S atoms of the bidentate piperidinecarbodithioate ligand occupying the vertices. The piperidine ring adopts a chair conformation.

Comment

Dithiocarbamate anions have proved to be highly versatile chelating agents for the separation of metals as metal chelates by gas chromatography (Riekkola *et al.*, 1979). Dithiocarbamate (dtc) ligands exhibit both bidentate behaviour, acting as *S*,*S*′-donors, and monodentate behaviour, acting as *S*-donors, depending on the type of complex (Forghieri *et al.*, 1988). Also, there has been a 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 serves to develop a better understanding of the luminescent properties of d^{10}–d^{10} systems (Yam *et al.*, 1990). Nevertheless, the number of reports on gold(I) complexes containing dtc anions and neutral ligands is quite limited. In this context, we present here the crystal structure of the title compound, (I).



(I)

The structure of (I) consists of mononuclear $[Au(Pipdtc)(PPh_3)_2]$ units (Pipdtc is piperidinecarbodithioate). The Au atom is in a distorted tetrahedral environment. This coordination is formed by two S atoms from the bidentate Pipdtc ligand, which forms a four-membered chelate ring, and two P atoms from the triphenylphosphine ligands. The angles around the Au atom range between 65.77 (8) and 130.86 (8)°. The smallest angle, which is S1—Au—S2, is due to the restricted bite angle of the ligand (Crespo *et al.*, 1997; Jones *et al.*, 1994; Gimeno *et al.*, 1994), whereas the largest angle, P1—Au—P2, is likely to arise in order to minimize steric interactions between the PPh_3 groups.

The four-membered AuS_2C ring is planar, with the maximum deviation from the plane being 0.018 (9) Å for C37. The Au1—S1 and S1—C37 bond lengths are longer than those of Au1—S2 and S2—C37, respectively. The shorter Au—S bond length (Au1—S2) lies adjacent to the C37—S2 bond, which is closer to the normal C═S bond length of 1.69 Å. This characteristic is also found and explained in detail in the complex $[Au(S_2CPh)(PPh_3)_2]$ (Lanfredi *et al.*, 1992).

The Au1—P1 and Au1—P2 distances are comparable with those found in the complex $[Au(S_2COEt)(PPh_3)_2]$ (Assefa *et al.*, 1994), but longer than the corresponding Ni—P distances of 2.201 (1) and 2.229 (1) Å found in the Ni analogue of (I) (Venkatachalam *et al.*, 1996). The C37—N1 bond length shows significant double-bond character, but is longer than that observed in the Ni analogue of (I) [2.284 (5) Å; Venkatachalam *et al.*, 1996]. The piperidine ring adopts a chair conformation. The total puckering amplitude Q_T is 0.54 (1) Å (Cremer & Pople, 1975).

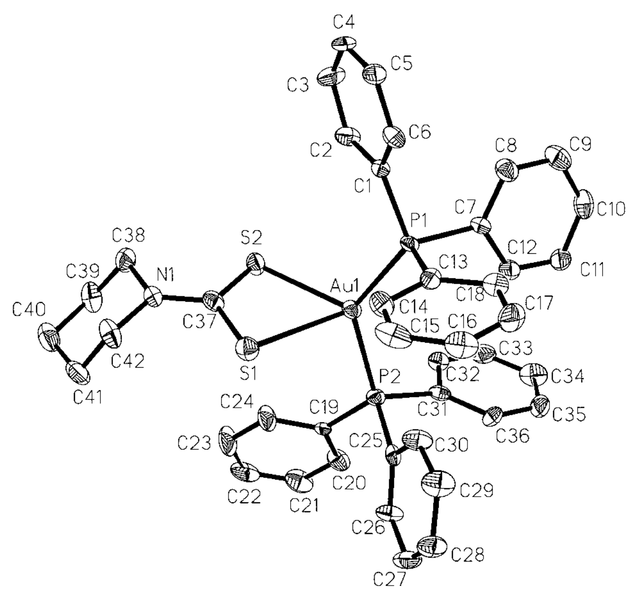


Figure 1
The structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms are omitted for clarity.

Experimental

Sodium piperidinecarbodithioate, $[Na(S_2CNC_5H_{10})]$, was dissolved in H_2O. Gold trichloride was added at room temperature with stirring. The brown reaction mixture was filtered and the filtrate was washed with water and dried overnight under vacuum. The dried filtrate was dissolved in EtOH and triphenylphosphine was added at 353–363 K with stirring. The solution was then refluxed for 4–5 h. Upon cooling, the light-yellow solution obtained was filtered and left to evaporate. After a few days, a light-yellow solid had separated out and was recrystallized from EtOH/$CHCl_3$. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an EtOH solution at room temperature (m.p. 424 K).

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Crystal data

$[Au(C_6H_{10}NS_2)(C_{18}H_{15}P)_2]$	$Z = 2$
$M_r = 881.78$	$D_x = 1.551$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 10.1318$ (2) Å	Cell parameters from 3234 reflections
$b = 13.2019$ (2) Å	$\theta = 2.88$–$28.35°$
$c = 14.9565$ (5) Å	$\mu = 4.123$ mm^{-1}
$\alpha = 77.207$ (1)°	$T = 293$ (2) K
$\beta = 80.992$ (2)°	Slab, colourless
$\gamma = 76.834$ (2)°	$0.46 \times 0.20 \times 0.12$ mm
$V = 1887.71$ (8) Å^3	

Data collection

Siemens SMART CCD area-detector diffractometer	6550 independent reflections
ω scans	4263 reflections with $I > 2\sigma(I)$
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.069$
$T_{min} = 0.253$, $T_{max} = 0.638$	$\theta_{max} = 25°$
10 680 measured reflections	$h = -12 \rightarrow 11$
	$k = -15 \rightarrow 15$
	$l = -17 \rightarrow 12$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0490P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.124$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.89$	$\Delta\rho_{max} = 1.65$ e Å^{-3}
6550 reflections	$\Delta\rho_{min} = -2.38$ e Å^{-3}
433 parameters	

Table 1
Selected geometric parameters (Å, °).

Au1—P1	2.336 (2)	S1—C37	1.731 (9)
Au1—P2	2.348 (2)	S2—C37	1.690 (10)
Au1—S2	2.561 (2)	N1—C37	1.357 (12)
Au1—S1	2.858 (3)		
P1—Au1—P2	130.86 (8)	P2—Au1—S1	98.80 (9)
P1—Au1—S2	112.26 (9)	S2—Au1—S1	65.77 (8)
P2—Au1—S2	115.94 (9)	C37—S1—Au1	82.2 (4)
P1—Au1—S1	109.05 (8)	C37—S2—Au1	92.6 (3)

After checking their presence in the difference map, all H atoms were geometrically fixed and allowed to ride on their attached atoms. The highest peak and deepest hole were found 1.25 and 1.00 Å, respectively, from the Au 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: LN1100). Services for accessing these data are described at the back of the journal.

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