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(4,6-Dimercapto-1,3,5-triazine-2-thiolato-S^2)tris(triphenylphosphine-*P*)-gold(I) dimethylformamide solvate

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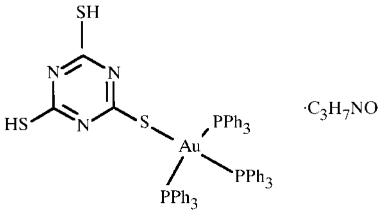
In the title compound, $[Au(C_3H_2N_3S_3)(C_{18}H_{15}P)_3]\cdot C_3H_7NO$, the Au^I atom has a distorted tetrahedral geometry consisting of one uncoordinated dimethylformamide molecule, one trithiocyanurate ligand and three PPh_3 ligands. The S—Au distance is 2.909 (2) Å, and the P—Au distances fall in the range 2.400 (14)–2.4074 (13) Å. The S—Au—P angles are 92.81 (6), 99.17 (6) and 104.21 (5)°, and the P—Au—P angles are 114.46 (5), 119.04 (5) and 119.66 (5)°.

Comment

There has been growing interest in the study of Cu^I, Ag^I and Au^I complexes, and in particular polynuclear systems; this stems from the tendency of these metal ions to form clusters and aggregates as a result of weak metal–metal interactions (Mingos, 1976; Schmidbaur, 1995) and the recent demonstration that a number of these aggregates exhibit rich luminescence behaviour (Vickery *et al.*, 1997; Yam *et al.*, 1999). Until now, Au^I–sulfido complexes have been comparatively rare (Canales *et al.*, 1994). Recently, an interesting example was found in studies of trigold(I) complexes of trithiocyanuric acid, in which an unexpected reaction led to formation of an interesting sheet structure through multiple intermolecular Au···Au-bonded self-assembly (William *et al.*, 1999). Also by use of Au^I, PPh_3 and trithiocyanuric acid, we obtained a different product, namely (4,6-dimercapto-1,3,5-triazine-2-thiolato-S^2)tris(triphenylphosphine-*P*)gold(I) dimethylformamide (DMF) solvate, (I), including a DMF molecule, one Au^I atom, one trithiocyanurate ligand and three PPh_3 ligands. In the crystal structure, only one thiolate of the trithiocyanuric acid has been coordinated to the Au^I atom and each Au^I is coordinated by one thiolate group of the trithiocyanurate ligand and three P atoms of the PPh_3 groups, giving a tetrahedral coordination. The S—Au distance is 2.909 (2) Å, which is much longer than the normal S—Au distance, and the P—Au distances fall in the range 2.400 (14)–2.4074 (13) Å. The S—Au—P angles are 92.81 (6), 99.17 (6) and 104.21 (5)°, and the P—Au—P angles are 114.46 (5), 119.04 (5) and 119.66 (5)°. Thus, the geometry is distorted tetrahedral.



(I)

Experimental

The title compound, (I), was obtained from the reaction of trithiocyanuric acid, PPh_3 and AuCN in DMF. To a solution of trithiocyanuric acid (0.5 mmol, 0.09 g) in DMF, AuCN (20 ml, 0.5 mmol, 0.12 g) and PPh_3 (1 mmol, 0.26 g) were added. After stirring for 2 h, the orange solution was filtered. Ether was diffused slowly into the filtrate solution. A week later, crystals suitable for X-ray diffraction analysis were obtained.

Crystal data

$[Au(C_3H_2N_3S_3)(C_{18}H_{15}P)_3]\cdot C_3H_7NO$
$M_r = 1233.13$
Triclinic, $P\overline{1}$
$a = 13.7053$ (12) Å
$b = 13.9751$ (12) Å
$c = 14.4614$ (12) Å
$\alpha = 80.665$ (2)°
$\beta = 87.283$ (2)°
$\gamma = 87.942$ (2)°
$V = 2729.0$ (4) Å^3
$Z = 2$
$D_x = 1.501$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 925 reflections
$\theta = 11.6$–18.9°
$\mu = 2.943$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.25 × 0.22 × 0.20 mm

Data collection

SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*XEMP* in *SHELXTL*; Sheldrick, 1997)
$T_{min} = 0.420$, $T_{max} = 0.555$
18 651 measured reflections
12 409 independent reflections
9513 reflections with $I > 2\sigma(I)$
$R_{int} = 0.0353$
$\theta_{max} = 27.56°$
$h = -17 \rightarrow 17$
$k = -18 \rightarrow 12$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.113$
$S = 0.967$
12 409 reflections
624 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.19$ e Å^{-3}
$\Delta\rho_{min} = -0.81$ e Å^{-3}

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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