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Key indicators

Single-crystal X-ray study

T = 105 K

Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$

R factor = 0.027

wR factor = 0.054

Data-to-parameter ratio = 35.6

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(2,4,6-Trimethyldithiobenzoato)(triphenylphosphine)gold(I)**

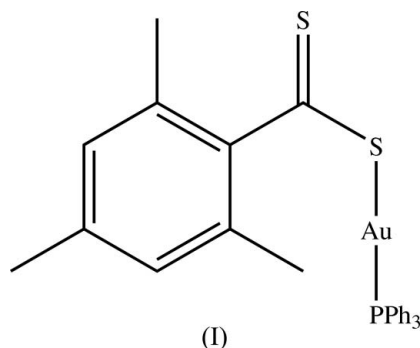
The title compound, $[\text{Au}(\text{C}_{10}\text{H}_{11}\text{S}_2)(\text{C}_{18}\text{H}_{15}\text{P})]$, features an Au^{I} atom linearly coordinated to a P atom and one S atom of the dithiobenzoate. The S—Au—P bond angle is $177.43(2)^\circ$. In contrast to other reported dithiobenzoate–gold complexes, in which the second S atom is *syn* with respect to Au, the title compound shows an uncoordinated S atom in an *anti* conformation.

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Comment

We recently reported (Macalindong *et al.*, 2006) the structure of a linear gold(I) complex with a triphenylphosphine ligand and 2-methyldithiobenzoate acting as a monodentate ligand. That complex is chemically similar to the title compound, (I), differing only in the ring substitution. The main structural difference lies in the Au—S—C—S torsion angles: $-174.0(1)^\circ$ in (I) (*anti* with respect to the Au atom) *versus* $-3.1(2)$ and $+0.2(2)^\circ$ in the two independent molecules [(II) and (III)] previously reported. It is also worth noting that few of the chemically equivalent structural parameters associated with the Au coordination environment in these three molecules show consistent statistical equivalence. Some examples, with values are listed in the order (I), (II), (III): P—Au [2.2623(6), 2.2568(6) and 2.2632(6) Å], Au—S [2.3155(6), 2.3240(6) and 2.3320(6) Å] and P—Au—S [$177.43(2)$, $175.03(2)$ and $173.83(2)^\circ$]. This suggests that these gold(I) complexes are not very rigid and are easily deformed by crystal packing forces.

**Experimental**

To a stirred solution of 0.5 g $[(n\text{-C}_3\text{H}_7)_4\text{N}][2,4,6\text{-(CH}_3)_3\text{C}_6\text{H}_2\text{CS}_2]$ in DMF (20 ml) was added $\text{NaAuCl}_4 \cdot 2\text{H}_2\text{O}$ (0.26 g) dissolved in DMF (10 ml). The pale-orange solution was stirred for 24 h and the resulting red-brown precipitate was filtered, washed with DMF and air dried. This solid (0.02 g) was dissolved in $\text{CS}_2\text{-CHCl}_3$ (16 ml, 1:1 *v/v*) and added to PPh_3 (0.014 g) dissolved in $\text{CS}_2\text{-CHCl}_3$ (2 ml, 1:1 *v/v*). This pink solution was evaporated and the resulting orange residue was washed with a 3:2 absolute ethanol/cyclohexane solution,

suction filtered and air dried. The orange solid was recrystallized from diethyl ether (Schuerman, 1988).

Crystal data

[Au(C₁₀H₁₁S₂)(C₁₈H₁₅P)]

$M_r = 654.54$

Monoclinic, $P2_1/n$

$a = 8.9954$ (10) Å

$b = 20.745$ (2) Å

$c = 13.553$ (2) Å

$\beta = 93.002$ (5)°

$V = 2525.6$ (5) Å³

$Z = 4$

$D_x = 1.721$ Mg m⁻³

Mo $K\alpha$ radiation

$\mu = 6.07$ mm⁻¹

$T = 105$ K

Fragment, orange

$0.20 \times 0.15 \times 0.12$ mm

Data collection

Nonius KappaCCD diffractometer

with an Oxford Cryosystems

Cryostream cooler

ω scans with κ offsets

Absorption correction: multi-scan

(SCALEPACK; Otwinowski &

Minor, 1997)

$T_{\min} = 0.431$, $T_{\max} = 0.530$

(expected range = 0.393–0.483)

48287 measured reflections

10430 independent reflections

8513 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\text{max}} = 34.3^\circ$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.054$

$S = 0.95$

10430 reflections

293 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0096P)^2$

$+ 5.4333P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.84$ e Å⁻³

$\Delta\rho_{\text{min}} = -1.26$ e Å⁻³

Extinction correction: SHELXL97

Extinction coefficient: 0.00059 (5)

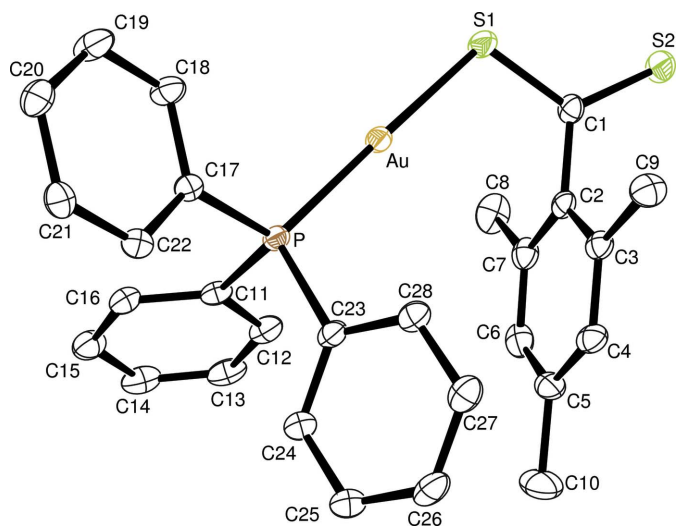


Figure 1

View of (I) (50% probability displacement ellipsoids). H atoms are not shown.

reduction: DENZO and SCALEPACK; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

The purchase of the diffractometer was made possible by Grant No. LEQSF(1999–2000)-ESH-TR-13, administered by the Louisiana Board of Regents.

Table 1

Selected geometric parameters (Å, °).

C1–S2	1.651 (2)	Au–P	2.2623 (6)
C1–S1	1.721 (2)	Au–S1	2.3155 (6)
S2–C1–S1	120.66 (15)	C1–S1–Au	104.07 (8)
P–Au–S1	177.43 (2)		

H atoms were placed in calculated positions, with C–H bond distances 0.95–0.98 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$, and thereafter treated as riding. A torsional parameter was refined for each methyl group. The deepest hole is located 0.67 Å from the Au atom.

Data collection: COLLECT (Nonius, 2000); cell refinement: DENZO and SCALEPACK (Otwinowski & Minor, 1997); data

References

- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Macalindong, J. S., Fronczek, F. R., Schuerman, J. A., Selbin, J. & Watkins, S. F. (2006). *Acta Cryst.* **E62**, m889–m890.
 Nonius (2000). 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.
 Schuerman, J. A. (1988). *Univ. Microfilms Int. Order No. DA8904565*. (1988), 345 pp. From: *Diss. Abstr. Int. B* (1989), **49**, Part 1, 5300–5301.
 Sheldrick, G. M. (1997). SHELXL97 and SHELXS97. University of Göttingen, Germany.