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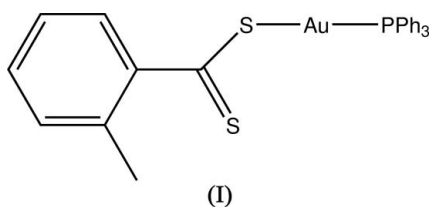
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**Key indicators**Single-crystal X-ray study  
 $T = 100$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.029  
 $wR$  factor = 0.063  
Data-to-parameter ratio = 34.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**(2-Methyldithiobenzoato- $\kappa$ S)(triphenylphosphine- $\kappa$ O)gold(I)**

The asymmetric unit of the title compound,  $o\text{-CH}_3(\text{C}_6\text{H}_4)\text{-C}(\text{S})\text{S-Au-P}(\text{C}_6\text{H}_5)_3$  or  $[\text{Au}(\text{C}_8\text{H}_7\text{S}_2)(\text{C}_{18}\text{H}_{15}\text{P})]$ , consists of two quasi-linear gold complexes. The S—Au—P bond angles [ $173.83(2)$ ,  $175.03(2)^\circ$ ], S—Au bond lengths [ $2.3240(6)$ ,  $2.3329(6)$  Å] and Au—P bond lengths [ $2.2568(6)$ ,  $2.2632(6)$  Å] are consistent with previously reported values. The major difference in the two molecules is that the  $o$ -methylphenyl rings are twisted with respect to the dithiocarboxyl planes by  $73.0(3)^\circ$  and  $46.6(3)^\circ$ , as measured by S—C—C torsion angles.

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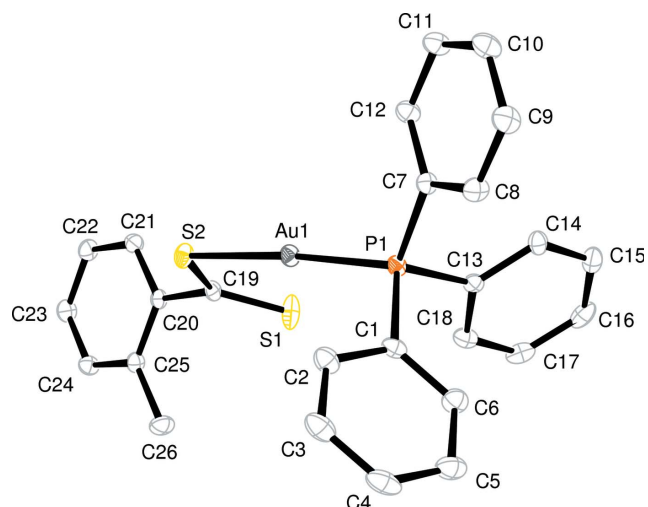
The  $o$ -methyldithiobenzoate anion most often coordinates as a bidentate ligand (Biagini-Cingi *et al.*, 1997; Kato *et al.*, 2000), and has been shown to act as a bridging ligand in an Au(I) hexamer (Schuerman *et al.*, 1986). This is the first reported instance of its monodentate coordination to a coinage metal. The dithiobenzoate ligand coordinates in monodentate fashion in the analogous compound lacking the methyl group,  $(\text{C}_6\text{H}_5\text{CS}_2)\text{AuP}(\text{C}_6\text{H}_5)_3$  (Manotti-Lanfredi *et al.*, 1992). In that structure, which also has two independent molecules, the Au—S distances are  $2.301(4)$  and  $2.338(3)$  Å, the Au—P distances are  $2.269(6)$  and  $2.263(4)$  Å, and the S—Au—P angles are slightly closer to linearity than in the title complex,  $177.2(3)$  and  $179.0(2)^\circ$ . The major difference in the two molecules of the asymmetric unit is that the  $o$ -methylphenyl rings are twisted with respect to the dithiocarboxyl planes by  $73.0(3)^\circ$  and  $46.6(3)^\circ$ , as measured by S—C—C—C torsion angles.



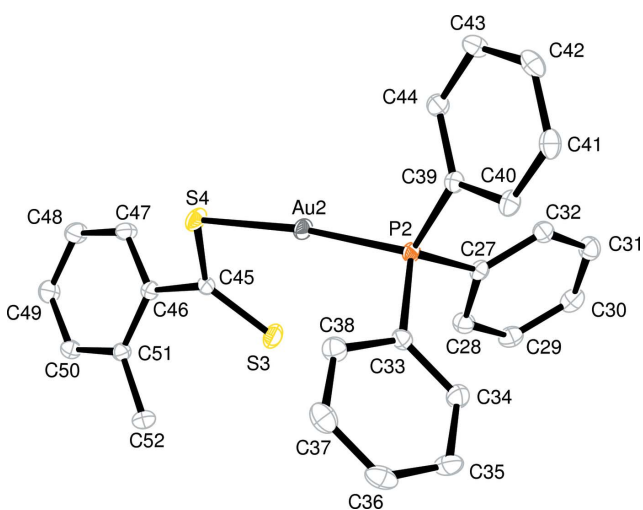
Cell dimensions of the title compound at 291 K, measured on an Enraf–Nonius CAD4 diffractometer with Mo  $K\alpha$  radiation, are  $a = 19.7028(10)$ ,  $b = 12.5068(14)$ ,  $c = 18.784(2)$  Å,  $\beta = 93.314(8)^\circ$ ,  $V = 4621.0(14)$  Å<sup>3</sup>.

**Experimental**

A solution of 0.0105 g  $\text{PPh}_3$  in 4 ml of  $\text{CS}_2$  was added to 0.0050 g  $[\text{Au}_6(\text{CH}_3\text{C}_6\text{H}_4\text{CS}_2)_6]$  (Schuerman *et al.*, 1986) dissolved in 4 ml  $\text{CS}_2$ . The pinkish–purple precipitate was filtered, air-dried, and recrystallized from diethyl ether (Schuerman, 1988).



**Figure 1**  
Molecule 1 of the asymmetric unit of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% level. H atoms are omitted.



**Figure 2**  
Molecule 2 of the asymmetric unit of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% level. H atoms are omitted.

#### Crystal data

[Au(C<sub>8</sub>H<sub>7</sub>S<sub>2</sub>)(C<sub>18</sub>H<sub>15</sub>P)]  
 $M_r = 626.49$   
 Monoclinic,  $P2_1/c$   
 $a = 19.525$  (2) Å  
 $b = 12.3297$  (10) Å  
 $c = 18.6250$  (10) Å  
 $\beta = 93.486$  (3)°  
 $V = 4475.4$  (6) Å<sup>3</sup>  
 $Z = 8$

#### Data collection

Nonius KappaCCD diffractometer  
 with Oxford Cryostream  
 $\omega$  scans with  $\kappa$  offsets  
 Absorption correction: multi-scan  
*HKL SCALEPACK*  
 (Otwinowski & Minor 1997)  
 $T_{\min} = 0.198$ ,  $T_{\max} = 0.256$   
 83707 measured reflections

$D_x = 1.86$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 17051  
 reflections  
 $\theta = 2.5$ – $35^\circ$   
 $\mu = 6.84$  mm<sup>-1</sup>  
 $T = 100$  K  
 Fragment, purple  
 0.28 × 0.24 × 0.20 mm

18706 independent reflections  
 15875 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$   
 $\theta_{\text{max}} = 35.0^\circ$   
 $h = -30 \rightarrow 31$   
 $k = -18 \rightarrow 19$   
 $l = -30 \rightarrow 30$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.063$   
 $S = 1.02$   
 18706 reflections  
 543 parameters  
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0199P)^2 + 8.6263P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.006$   
 $\Delta\rho_{\text{max}} = 3.06 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -1.63 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Au1—P1	2.2568 (6)	Au2—P2	2.2632 (6)
Au1—S2	2.3240 (6)	Au2—S4	2.3329 (6)
S1—C19	1.648 (2)	S3—C45	1.645 (2)
S2—C19	1.716 (2)	S4—C45	1.734 (2)
C19—C20	1.492 (3)	C45—C46	1.496 (3)
P1—Au1—S2	175.03 (2)	P2—Au2—S4	173.83 (2)
C19—S2—Au1	101.06 (8)	C45—S4—Au2	101.31 (8)
C20—C19—S1	119.84 (17)	C46—C45—S3	121.71 (17)
C20—C19—S2	113.59 (16)	C46—C45—S4	114.35 (16)
S1—C19—S2	126.57 (13)	S3—C45—S4	123.93 (14)
S1—C19—C20—C25	73.0 (3)	S3—C45—C46—C51	46.6 (3)

H atoms were placed in calculated positions, guided by difference maps, with C—H bond distances 0.95–0.98 Å,  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$  (1.5 for methyl), and thereafter refined as riding. A torsional parameter was refined for each methyl group. The largest residual peak is located 1.04 Å from Au1, and all peaks with density greater than  $1 \text{ e \AA}^{-3}$  are located within 1.11 Å of Au positions. The deepest hole is located 0.56 from atom Au2.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO* (Otwinowski & Minor 1997) 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: *SHELXL97*.

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