

Refinement

Refinement on F

R = 0.032

wR = 0.032

S = 0.53

4295 reflections

273 parameters

Only H-atom U's refined

Unit weights applied

 $(\Delta/\sigma)_{\max} = 0.004$

$$\Delta\rho_{\max} = 0.48 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$$

Extinction correction:

Zachariasen (1967)

Extinction coefficient:

0.42 (1) (length in mm)

Atomic scattering factors

from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Cu—O(1)—Cl(1)	124.7 (1)	N(3)—C(9)—C(8)	113.0 (2)
Cu—O(5)—Cl(2)	132.3 (1)	C(4)—C(9)—C(8)	111.4 (2)
Cu—N(1)—C(1)	118.7 (2)	N(3)—C(10)—C(11)	112.2 (2)
Cu—N(2)—C(3)	117.7 (1)	C(10)—C(11)—C(12)	114.5 (2)
Cu—N(2)—C(4)	107.1 (1)	N(4)—C(12)—C(11)	111.8 (2)
C(3)—N(2)—C(4)	112.5 (2)		

The structure was solved by direct and Fourier methods and refined by full-matrix least-squares techniques. H atoms were located by difference Fourier methods. *NRCVAX* (Gabe, Le Page, White & Lee, 1987) was used for all calculations.

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Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

$$B_{\text{eq}} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*a_i\cdot a_j$$

	x	y	z	B_{eq}
Cu	0.89377 (3)	0.74711 (3)	0.25802 (2)	1.817 (9)
Cl(1)	0.78292 (7)	0.69847 (7)	-0.00307 (5)	2.65 (2)
Cl(2)	0.96878 (7)	0.77767 (7)	0.54090 (5)	2.89 (2)
O(1)	0.9136 (2)	0.7143 (3)	0.04523 (17)	3.86 (10)
O(2)	0.8445 (3)	0.6551 (3)	-0.12043 (16)	4.64 (12)
O(3)	0.7139 (4)	0.5950 (3)	0.0559 (2)	6.15 (16)
O(4)	0.6601 (3)	0.8353 (3)	0.0107 (2)	5.61 (12)
O(5)	0.8632 (3)	0.8219 (3)	0.46432 (17)	4.15 (10)
O(6)	1.1357 (3)	0.7390 (3)	0.4798 (2)	6.01 (14)
O(7)	0.9337 (4)	0.6560 (3)	0.5967 (3)	6.81 (16)
O(8)	0.9342 (4)	0.8913 (4)	0.6237 (2)	6.89 (16)
N(1)	1.1335 (2)	0.6360 (2)	0.23508 (19)	2.77 (8)
N(2)	0.9379 (2)	0.94103 (19)	0.22683 (15)	1.82 (6)
N(3)	0.6518 (2)	0.86429 (19)	0.28348 (15)	1.79 (6)
N(4)	0.8347 (3)	0.5603 (2)	0.28752 (19)	2.70 (8)
C(1)	1.2550 (3)	0.6799 (3)	0.1471 (2)	2.91 (9)
C(2)	1.2429 (3)	0.8371 (3)	0.1642 (2)	2.93 (10)
C(3)	1.0890 (3)	0.9414 (3)	0.1410 (2)	2.75 (10)
C(4)	0.7869 (3)	1.0412 (2)	0.20154 (17)	1.84 (8)
C(5)	0.7830 (3)	1.2002 (3)	0.2010 (2)	2.67 (10)
C(6)	0.6209 (3)	1.2961 (3)	0.1816 (2)	3.09 (11)
C(7)	0.4764 (3)	1.2768 (3)	0.2695 (3)	3.27 (11)
C(8)	0.4790 (3)	1.1184 (3)	0.2688 (2)	2.91 (10)
C(9)	0.6407 (3)	1.0210 (2)	0.28856 (17)	1.84 (7)
C(10)	0.5369 (3)	0.8264 (3)	0.3808 (2)	2.38 (9)
C(11)	0.5381 (3)	0.6697 (3)	0.3702 (2)	2.82 (10)
C(12)	0.6945 (3)	0.5610 (3)	0.3830 (2)	2.77 (10)

Table 2. Selected geometric parameters (\AA , $^\circ$)

Cu—O(1)	2.555 (2)	N(4)—C(12)	1.481 (3)
Cu—O(5)	2.534 (2)	C(1)—C(2)	1.503 (4)
Cu—N(1)	2.018 (2)	C(2)—C(3)	1.513 (4)
Cu—N(2)	2.035 (2)	C(4)—C(5)	1.526 (3)
Cu—N(3)	2.046 (2)	C(4)—C(9)	1.522 (3)
Cu—N(4)	2.024 (2)	C(5)—C(6)	1.521 (4)
N(1)—C(1)	1.479 (3)	C(6)—C(7)	1.513 (4)
N(2)—C(3)	1.487 (3)	C(7)—C(8)	1.523 (4)
N(2)—C(4)	1.488 (3)	C(8)—C(9)	1.525 (3)
N(3)—C(9)	1.489 (3)	C(10)—C(11)	1.516 (3)
N(3)—C(10)	1.484 (3)	C(11)—C(12)	1.504 (4)
O(1)—Cu—O(5)	170.98 (8)	Cu—N(3)—C(9)	108.2 (1)
O(1)—Cu—N(1)	90.36 (8)	Cu—N(3)—C(10)	116.4 (1)
O(1)—Cu—N(2)	87.40 (7)	C(9)—N(3)—C(10)	112.4 (2)
O(1)—Cu—N(3)	90.56 (7)	Cu—N(4)—C(12)	118.3 (2)
O(1)—Cu—N(4)	91.54 (8)	N(1)—C(1)—C(2)	111.8 (2)
O(5)—Cu—N(1)	93.77 (8)	C(1)—C(2)—C(3)	114.4 (2)
O(5)—Cu—N(2)	84.32 (8)	N(2)—C(3)—C(2)	112.9 (2)
O(5)—Cu—N(3)	85.14 (7)	N(2)—C(4)—C(5)	114.5 (2)
O(5)—Cu—N(4)	96.50 (9)	N(2)—C(4)—C(9)	107.4 (2)
N(1)—Cu—N(2)	94.01 (8)	C(5)—C(4)—C(9)	110.7 (2)
N(1)—Cu—N(3)	178.45 (8)	C(4)—C(5)—C(6)	111.2 (2)
N(1)—Cu—N(4)	89.63 (9)	C(5)—C(6)—C(7)	111.5 (2)
N(2)—Cu—N(3)	84.79 (7)	C(6)—C(7)—C(8)	110.3 (2)
N(2)—Cu—N(4)	176.21 (8)	C(7)—C(8)—C(9)	111.1 (2)
N(3)—Cu—N(4)	91.59 (8)	N(3)—C(9)—C(4)	107.7 (2)

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71649 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS1069]

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Benzenethiolato(triphenylphosphine)gold(I)

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Abstract

The crystal structure of [Au(C₆H₅S)(C₁₈H₁₅P)] contains two Au^I centers; each Au^I is almost linearly coordinated [P—Au—S bond angles of 179.0 (1) and

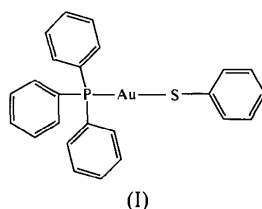
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175.9 (1)°] and an Au^I...Au^I intramolecular distance of 3.154 (2) Å is found.

Comment

Gold(I) compounds with sulfur-containing ligands are used in the treatment of rheumatoid arthritis (Brown & Smith, 1980). This chemistry has been expanded to include phosphine-sulfur gold complexes by the development of Auranofin as a successful drug (Parish & Cottrill, 1987). As part of our continuing effort to understand the basic chemistry of gold(I)-sulfur compounds, we have determined the structure of [Au(SPh)(PPh₃)] (I), which was prepared by the method reported by Baenziger, Dittmore & Doyle (1974). The structure of the compound is shown in Fig. 1.



Gold(I) phosphite-sulfur complexes are numerous. Several related structures have been compared by Muir, Cuadrado & Muir (1988), where the description of (2-benzoxazolethiolato)(triphenylphosphine)-gold(I), [Au(Sboz)(PPh₃)], was presented and compared with related complexes. Cookson & Tiekink (1993) have compared various gold(I) alkylsulfur-phosphine complexes and found that the crystallization of these complexes was not in dinuclear fragments with short Au...Au interactions. Specifically, the related (2-pyridinethiolato)(triphenylphosphine)gold(I) compound, [Au(2-Spy)(PPh₃)], crystallized with an Au...Au interaction distance of 5.673 (1) Å.

We have reported previously the structure of the gold(III) benzenethiolato complex [Au₂Cl₄(μ-SPh)] (Wang & Fackler, 1990). The gold(III) complex showed the ease with which gold(I) complexes dimerize to form gold(III) thiol-bridged species. We now report the structure of [Au(SPh)(PPh₃)], which crystallizes with an Au...Au separation of 3.154 (2) Å, with the S atoms remaining strictly monodentate. This distance is longer than that of the gold(III) complex [3.077 (3) Å]. The P—Au—S angles of 179.0 (1) and 175.9 (1)° are essentially linear. Crane & Beall (1978) stated that a P—Au—S angle of 173.5° is evidence of Au...Au attractions, although exceptions have been found (Cookson & Tiekink, 1993). The angles and the Au...Au interaction reported here for [Au(SPh)(PPh₃)] agree with this observation. Although the gold center is not

formally three-coordinate, three-coordinate gold(I) centers are known for bis(phosphine)gold(I) halides and SCN complexes (Staples, King, Khan, Winpenny & Fackler, 1993). We are also aware of a few examples involving gold(I) with phosphines and bidentate sulfur chelate ligands (Dávila, Elduque, Grant, Staples & Fackler, 1993).

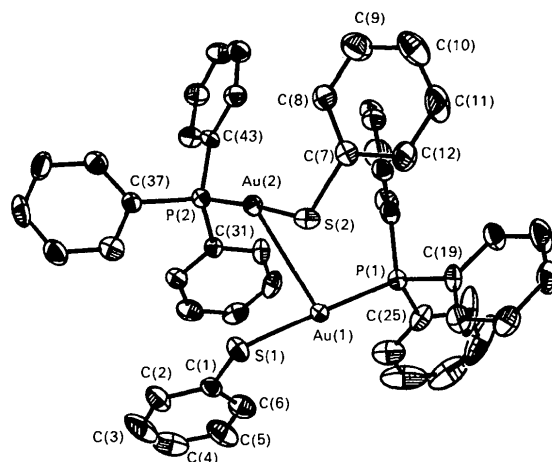


Fig. 1. A drawing of the two molecules of [Au(SPh)(PPh₃)], showing the atomic labeling scheme with displacement ellipsoids drawn at 50% probability. The Au(1)...Au(2) distance is 3.154 (2) Å.

Experimental

Crystal data

[Au(C₆H₅S)(C₁₈H₁₅P)]₂

M_r = 1136.86

Triclinic

*P*1̄

a = 11.062 (5) Å

b = 11.616 (5) Å

c = 16.817 (6) Å

α = 97.15 (3)°

β = 93.45 (3)°

γ = 93.20 (3)°

V = 2136 (1) Å³

Z = 2

D_x = 1.77 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 25 reflections

θ = 25–30°

μ = 7.05 mm⁻¹

T = 293 K

0.2 × 0.15 × 0.08 mm

Colorless

Crystal source: CH₂Cl₂/Et₂O

Data collection

*R*3*m*/*E* diffractometer

Wyckoff scans

Absorption correction:

empirical

*T*_{min} = 0.32, *T*_{max} = 0.96

6106 measured reflections

5566 independent reflections

4352 observed reflections

[*F*_o² > 3σ(*F*_o²)]

θ_{max} = 25°

h = 0 → 12

k = -13 → 13

l = -19 → 19

3 standard reflections

monitored every 97

reflections

intensity variation: <1%

Refinement

Refinement on *F*²*R* = 0.0380*wR* = 0.0396*S* = 1.28

4352 reflections

484 parameters

H-atom parameters not refined

$$w = 1/[\sigma^2(F_o) + 0.00102F_o^2]$$

$$(\Delta/\sigma)_{\max} = 0.014$$

$$\Delta\rho_{\max} = 0.76 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -0.78 \text{ e } \text{Å}^{-3}$$

Atomic scattering factors
from *International Tables*
for *X-ray Crystallography*
(1974, Vol. IV)

Table 2. Geometric parameters (Å, °)

Au(1)—S(1)	2.318 (3)	C(9)—C(10)	1.37 (2)
Au(2)—S(2)	2.316 (3)	C(11)—C(12)	1.392 (18)
S(1)—C(1)	1.778 (11)	C(13)—C(18)	1.423 (16)
P(1)—C(13)	1.828 (10)	C(15)—C(16)	1.37 (2)
P(1)—C(25)	1.837 (11)	C(17)—C(18)	1.383 (16)
P(2)—C(37)	1.808 (11)	C(19)—C(24)	1.428 (17)
C(1)—C(2)	1.369 (17)	C(21)—C(22)	1.39 (2)
C(2)—C(3)	1.43 (2)	C(23)—C(24)	1.377 (19)
C(4)—C(5)	1.40 (3)	C(25)—C(30)	1.37 (2)
C(7)—C(8)	1.373 (15)	C(27)—C(28)	1.33 (3)
C(8)—C(9)	1.386 (19)	C(28)—C(29)	1.37 (3)
C(10)—C(11)	1.362 (19)	C(31)—C(32)	1.379 (14)
C(13)—C(14)	1.383 (14)	C(32)—C(33)	1.388 (14)
C(14)—C(15)	1.371 (14)	C(34)—C(35)	1.352 (18)
C(16)—C(17)	1.36 (2)	C(37)—C(38)	1.403 (15)
C(19)—C(20)	1.381 (16)	C(38)—C(39)	1.411 (18)
C(20)—C(21)	1.395 (17)	C(40)—C(41)	1.380 (19)
C(22)—C(23)	1.38 (2)	C(43)—C(44)	1.405 (14)
C(25)—C(26)	1.382 (18)	C(44)—C(45)	1.381 (16)
C(26)—C(27)	1.389 (18)	C(46)—C(47)	1.336 (17)
Au(1)—P(1)	2.278 (3)	C(29)—C(30)	1.40 (2)
Au(2)—P(2)	2.269 (3)	C(31)—C(36)	1.383 (14)
S(2)—C(7)	1.761 (10)	C(33)—C(34)	1.385 (18)
P(1)—C(19)	1.814 (11)	C(35)—C(36)	1.421 (13)
P(2)—C(31)	1.813 (8)	C(37)—C(42)	1.394 (14)
P(2)—C(43)	1.830 (9)	C(39)—C(40)	1.372 (17)
C(1)—C(6)	1.422 (16)	C(41)—C(42)	1.403 (18)
C(3)—C(4)	1.25 (2)	C(43)—C(48)	1.362 (14)
C(5)—C(6)	1.345 (19)	C(45)—C(46)	1.362 (17)
C(7)—C(12)	1.411 (16)	C(47)—C(48)	1.446 (15)
S(1)—Au(1)—P(1)	179.0 (1)	P(1)—C(19)—C(20)	119.5 (9)
Au(1)—S(1)—C(1)	108.6 (4)	C(20)—C(19)—C(24)	118.8 (10)
Au(1)—P(1)—C(13)	112.3 (4)	C(20)—C(21)—C(22)	119.4 (12)
C(13)—P(1)—C(19)	105.5 (5)	C(22)—C(23)—C(24)	119.5 (13)
C(13)—P(1)—C(25)	106.7 (5)	P(1)—C(25)—C(26)	117.8 (10)
Au(2)—P(2)—C(31)	114.0 (3)	C(26)—C(25)—C(30)	119.9 (11)
C(31)—P(2)—C(37)	106.5 (4)	C(26)—C(27)—C(28)	128.1 (15)
C(31)—P(2)—C(43)	102.3 (4)	C(28)—C(29)—C(30)	122.3 (18)
S(1)—C(1)—C(2)	118.7 (9)	P(2)—C(31)—C(32)	118.4 (7)
C(2)—C(1)—C(6)	117.5 (11)	C(32)—C(31)—C(36)	118.6 (8)
C(2)—C(3)—C(4)	123.9 (17)	C(32)—C(33)—C(34)	118.7 (11)
C(4)—C(5)—C(6)	116.9 (13)	C(34)—C(35)—C(36)	121.4 (11)
S(2)—C(7)—C(8)	124.7 (9)	P(2)—C(37)—C(38)	119.0 (8)
C(8)—C(7)—C(12)	117.0 (10)	C(38)—C(37)—C(42)	117.7 (10)
C(8)—C(9)—C(10)	120.8 (12)	C(38)—C(39)—C(40)	120.3 (11)
C(10)—C(11)—C(12)	121.1 (13)	C(40)—C(41)—C(42)	118.8 (11)
P(1)—C(13)—C(14)	119.1 (8)	P(2)—C(43)—C(44)	119.9 (7)
C(14)—C(13)—C(18)	117.8 (9)	C(44)—C(43)—C(48)	119.6 (9)
C(14)—C(15)—C(16)	121.4 (11)	C(44)—C(45)—C(46)	121.4 (11)
C(16)—C(17)—C(18)	121.7 (13)	C(46)—C(47)—C(48)	120.4 (10)
S(2)—Au(2)—P(2)	175.9 (1)	P(1)—C(19)—C(24)	121.7 (8)
Au(2)—S(2)—C(7)	107.7 (3)	C(19)—C(20)—C(21)	120.5 (11)
Au(1)—P(1)—C(19)	113.3 (4)	C(21)—C(22)—C(23)	121.3 (12)
Au(1)—P(1)—C(25)	113.1 (4)	C(19)—C(24)—C(23)	120.4 (11)
C(19)—P(1)—C(25)	105.4 (5)	P(1)—C(25)—C(30)	123.3 (10)
Au(2)—P(2)—C(37)	110.6 (3)	C(25)—C(26)—C(27)	119.4 (14)
Au(2)—P(2)—C(43)	115.4 (3)	C(27)—C(28)—C(29)	117.3 (14)
P(1)—P(2)—C(43)	107.2 (4)	C(25)—C(30)—C(28)	118.9 (7)
S(1)—C(1)—C(6)	123.8 (9)	P(2)—C(31)—C(36)	123.0 (7)
C(1)—C(2)—C(3)	117.0 (12)	C(31)—C(32)—C(33)	122.4 (10)
C(3)—C(4)—C(5)	121.8 (16)	C(33)—C(34)—C(35)	120.0 (10)
C(1)—C(6)—C(5)	122.9 (13)	C(31)—C(36)—C(35)	118.9 (10)
S(2)—C(7)—C(12)	118.3 (8)	P(2)—C(37)—C(42)	123.2 (8)
C(7)—C(8)—C(9)	121.8 (12)	C(37)—C(38)—C(39)	120.1 (10)
C(9)—C(10)—C(11)	118.8 (13)	C(39)—C(40)—C(41)	120.9 (12)
C(7)—C(12)—C(11)	120.4 (10)	C(37)—C(42)—C(41)	122.1 (11)
P(1)—C(13)—C(18)	122.9 (7)	P(2)—C(43)—C(48)	120.5 (7)
C(13)—C(14)—C(15)	120.9 (10)	C(43)—C(44)—C(45)	119.4 (10)
C(15)—C(16)—C(17)	119.0 (11)	C(45)—C(46)—C(47)	120.2 (11)
C(13)—C(18)—C(17)	119.1 (11)	C(43)—C(48)—C(47)	118.9 (10)

The phenyl-ring atoms C20–C30 show large displacement ellipsoids, which suggest that the rings might be disordered. However, attempts to successfully model this potential disorder failed to improve the model's statistics. Calculations were performed

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)

$$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
Au(1)	0.2653 (1)	0.0922 (1)	0.1780 (1)	0.038 (1)
Au(2)	0.4259 (1)	0.2296 (1)	0.3245 (1)	0.037 (1)
S(1)	0.2987 (2)	−0.0508 (2)	0.2599 (2)	0.050 (1)
S(2)	0.5634 (2)	0.1791 (2)	0.2296 (2)	0.048 (1)
P(1)	0.2319 (2)	0.2304 (2)	0.0956 (2)	0.041 (1)
P(2)	0.2916 (2)	0.2661 (2)	0.4199 (2)	0.036 (1)
C(1)	0.1560 (10)	−0.1094 (8)	0.2848 (6)	0.049 (4)
C(2)	0.1519 (11)	−0.1679 (10)	0.3505 (8)	0.068 (5)
C(3)	0.0359 (17)	−0.2167 (12)	0.3670 (11)	0.106 (8)
C(4)	−0.0596 (13)	−0.2096 (13)	0.3250 (12)	0.093 (8)
C(5)	−0.0616 (13)	−0.1494 (12)	0.2576 (11)	0.091 (7)
C(6)	0.0450 (10)	−0.1019 (10)	0.2390 (8)	0.068 (5)
C(7)	0.6462 (8)	0.3072 (9)	0.2137 (6)	0.042 (4)
C(8)	0.6823 (10)	0.3973 (11)	0.2727 (7)	0.061 (5)
C(9)	0.7526 (12)	0.4933 (12)	0.2570 (9)	0.082 (6)
C(10)	0.7904 (11)	0.5009 (12)	0.1815 (9)	0.086 (6)
C(11)	0.7569 (12)	0.4125 (12)	0.1218 (8)	0.083 (6)
C(12)	0.6828 (11)	0.3173 (11)	0.1358 (7)	0.066 (5)
C(13)	0.2474 (9)	0.3775 (9)	0.1499 (6)	0.047 (4)
C(14)	0.3611 (9)	0.4236 (9)	0.1803 (6)	0.048 (4)
C(15)	0.3757 (12)	0.5310 (10)	0.2252 (7)	0.063 (5)
C(16)	0.2786 (14)	0.5953 (11)	0.2424 (8)	0.079 (6)
C(17)	0.1652 (13)	0.5511 (11)	0.2144 (8)	0.080 (6)
C(18)	0.1461 (11)	0.4440 (10)	0.1680 (7)	0.065 (5)
C(19)	0.3371 (9)	0.2306 (10)	0.0170 (6)	0.052 (4)
C(20)	0.3818 (10)	0.1272 (10)	−0.0147 (7)	0.060 (5)
C(21)	0.4569 (10)	0.1241 (11)	−0.0785 (7)	0.071 (5)
C(22)	0.4932 (11)	0.2272 (12)	−0.1066 (7)	0.077 (6)
C(23)	0.4511 (13)	0.3320 (13)	−0.0756 (8)	0.092 (7)
C(24)	0.3742 (10)	0.3350 (10)	−0.0140 (7)	0.064 (5)
C(25)	0.0800 (10)	0.2129 (11)	0.0433 (7)	0.061 (5)
C(26)	−0.0052 (10)	0.1377 (11)	0.0699 (9)	0.079 (6)
C(27)	−0.1227 (11)	0.1266 (14)	0.0344 (13)	0.133 (9)
C(28)	−0.1564 (13)	0.1804 (17)	−0.0280 (10)	0.133 (9)
C(29)	−0.0720 (15)	0.2549 (22)	−0.0542 (9)	0.171 (12)
C(30)	0.0469 (13)	0.2729 (19)	−0.0192 (9)	0.139 (10)
C(31)	0.1363 (7)	0.2164 (8)	0.3869 (6)	0.037 (3)
C(32)	0.0832 (8)	0.2585 (10)	0.3209 (6)	0.051 (4)
C(33)	−0.0362 (10)	0.2280 (7)	0.2927 (7)	0.065 (5)
C(34)	−0.1045 (9)	0.1523 (10)	0.3323 (7)	0.061 (5)
C(35)	−0.0533 (10)	0.1115 (10)	0.3980 (8)	0.066 (5)
C(36)	0.0673 (8)	0.1418 (9)	0.4266 (7)	0.048 (4)
C(37)	0.3309 (7)	0.1952 (8)	0.5068 (6)	0.038 (3)
C(38)	0.3416 (9)	0.0745 (10)	0.4967 (7)	0.057 (4)
C(39)	0.3762 (10)	0.0176 (10)	0.5631 (7)	0.066 (5)
C(40)	0.3971 (9)	0.0793 (11)	0.6382 (8)	0.072 (5)
C(41)	0.3876 (10)	0.1980 (12)	0.6500 (7)	0.071 (5)
C(42)	0.3537 (8)	0.2547 (10)	0.5839 (7)	0.054 (4)
C(43)	0.2775 (8)	0.4199 (8)	0.4555 (6)	0.037 (3)
C(44)	0.1804 (9)	0.4535 (10)	0.5014 (7)	0.054 (4)
C(45)	0.1721 (10)	0.5695 (10)	0.5293 (7)	0.061 (5)
C(46)	0.2575 (11)	0.6520 (10)	0.5148 (8)	0.066 (5)
C(47)	0.3509 (10)	0.6221 (10)	0.4716 (7)	0.060 (5)
C(48)	0.3622 (9)	0.5021 (9)	0.4395 (7)	0.053 (4)

using *SHELXTL* (Sheldrick, 1978) on a data General Eclipse 140 computer.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and torsion angles, along with a crystal packing diagram, have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71605 (43 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR1067]

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(*o*-Methoxybenzenethiolato)(triphenylphosphine)gold(I) Diethyl Ether Solvate

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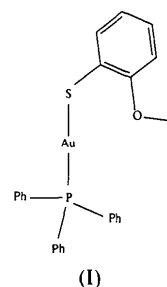
Abstract

The crystal structure of $[\text{Au}(\text{C}_7\text{H}_7\text{OS})(\text{C}_{18}\text{H}_{15}\text{P})] \cdot 0.25\text{C}_4\text{H}_{10}\text{O}$ contains two Au^{I} centers; each Au^{I} is almost linearly coordinated [P—Au—S bond angles of 175.2 (1) and 176.2 (1)°] and a large $\text{Au}^{\text{I}} \cdots \text{Au}^{\text{I}}$ intramolecular distance of 5.741 (3) Å is found.

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Comment

Gold(I) compounds with sulfur-containing ligands are used in the treatment of rheumatoid arthritis (Brown & Smith, 1980). This chemistry has been expanded to include phosphine–sulfur gold complexes through the development of Auranofin as a successful drug (Parish & Cottrill, 1987). As part of our continuing effort to understand the basic chemistry of gold(I)–sulfur compounds, we have determined the structure of $[\text{Au}(\text{PPh}_3)(\text{SPh-}o\text{-OMe})]$ (I). Compound (I) was prepared by the method reported by Baenziger, Dittmore & Doyle (1974). The compound is shown in Fig. 1.



Compound (I) crystallizes with an $\text{Au} \cdots \text{Au}$ separation of 5.741 (3) Å and P—Au—S angles showing linear geometry [175.2 (1) and 176.2 (1)°]. We have determined (Fackler, Staples, Elduque & Grant, 1994) the structure of $[\text{Au}(\text{SPh})(\text{PPh}_3)]$ which crystallized in dinuclear fragments with an $\text{Au} \cdots \text{Au}$ interaction of 3.154 (2) Å and P—Au—S angles of 179.0 (1) and 175.9 (1)°. Some related structures have been compared by Muir, Cuadrado & Muir (1988), in their report of the structure of (2-benzoxazolethiolato)(triphenylphosphine)gold(I), $[\text{Au}(\text{Sboz})\text{-(PPh}_3)]$.

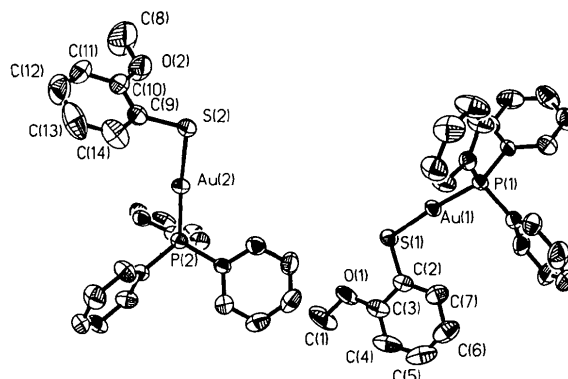


Fig. 1. A drawing of the two molecules of $[\text{Au}(\text{PPh}_3)\text{SPh-}o\text{-OMe}]$, showing the atomic labeling scheme with displacement ellipsoids drawn at 50% probability. The $\text{Au}(1) \cdots \text{Au}(2)$ distance is 5.741 (2) Å.