

References

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Benzoato(triphenylphosphine)gold(I) Benzene Solvate,* [Au(C₇H₅O₂){P(C₆H₅)₃].C₆H₆

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Abstract. $M_r = 658.49$, monoclinic, $P2_1/n$, $a = 10.825$ (2), $b = 13.896$ (3), $c = 17.411$ (4) Å, $\beta = 94.43$ (2)°, $V = 2611$ (2) Å³, $Z = 4$, $D_x = 1.675$ (2) g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 57$ cm⁻¹, $F(000) = 1288$, $T = 293$ K, $R = 0.042$ for 3433 observed reflections. The linear coordination at gold is slightly distorted [P–Au–O 173.7 (2)°]. The pattern of bond lengths, compared with the analogous acetate, can be explained by postulating better π -acceptor properties for benzoate. The benzene of solvation is well ordered and occupies holes in the lattice without participation in stacking interactions.

Introduction. As part of our study of gold carboxylate complexes, the title compound was synthesized [from Ph₃PAuCl and silver(I) benzoate] and recrystallized from benzene as colourless prisms. Elemental analysis suggested the presence of benzene of crystallization. The crystals slowly disintegrate when exposed to air, presumably by loss of benzene, and so were sealed in glass capillaries for structure determination.

Experimental. Crystal 0.5 × 0.25 × 0.05 mm, elongated along **b**, 5833 profile-fitted intensities (Clegg, 1981) measured on a Stoe-Siemens four-circle diffractometer; monochromated Mo $K\alpha$ radiation, $2\theta_{\text{max}} 50^\circ$, quadrant $-h + k \pm l$ ($|h| \leq 12$, $|k| \leq 16$, $|l| \leq 20$) and some $+h$ equivalents; three check reflections, no

intensity change; empirical absorption correction (ψ scans, transmissions 0.60–0.97); averaging equivalents gave 4587 unique reflections ($R_{\text{int}} 0.021$), 3433 with $F > 4\sigma(F)$ used for all calculations; cell constants refined from 2θ values of 36 reflections in range 20–23°; structure solution by heavy-atom method; refinement on $|F|$ to $R 0.042$, $wR 0.037$ [non-H atoms anisotropic, H atoms included using riding model with C–H 0.96 Å, $U(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]; 317 parameters, $w^{-1} = \sigma^2(F) + 0.00015F^2$, $S = 1.23$, slope of normal probability plot = 1.1], max. $\Delta/\sigma < 0.01$, max. and min. heights in final $\Delta\rho$ map +0.6, –0.8 e Å⁻³. Calculations with program system *SHELXTL* (Sheldrick, 1978). Atomic scattering factors those of Sheldrick (1981).

Discussion. Final atomic coordinates and derived parameters are given in Tables 1 and 2.† The gold atom shows the expected linear coordination (Fig. 1), albeit slightly distorted, with P–Au–O(1) 173.7 (2)°; the Au...O(2) contact of 3.037 (8) Å is too long to be regarded as an appreciable bonding interaction. Compared with the corresponding acetate (Jones, 1984), the following marginally significant changes are noted in the bond lengths of the PAuOCO group: Au–O(1) is shorter [2.033 (6) Å in the benzoate, 2.063 (6) Å in the

† Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and bond angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42122 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

* Carboxylate and Related Complexes of Gold. 3. Part 2: Jones (1984).

acetate], Au—P longer [2.213 (3), 2.207 (3) Å], C(1)—O(1) longer [1.297 (10), 1.268 (9) Å] and C(1)—O(2) longer [1.232 (10), 1.195 (12) Å]. This is consistent with regarding the benzoate π^* orbitals as better acceptors of electron density from the d^{10} metal atom; the aromatic ring is approximately coplanar with the PAuO₂ group [dihedral angle 8.4 (2)°].

Table 1. Atom coordinates ($\times 10^4$) and equivalent isotropic temperature factors ($\text{Å}^2 \times 10^3$)

	$U_{\text{eq}} = \frac{1}{3}$ (trace of orthogonalized U tensor).			
	x	y	z	U_{eq}
Au	6508 (1)	5918 (1)	6968 (1)	49 (1)
P	8172 (2)	6115 (1)	7773 (1)	43 (1)
O(1)	5074 (4)	5827 (4)	6145 (3)	63 (2)
O(2)	3729 (5)	6184 (4)	7008 (3)	68 (2)
C(1)	3973 (7)	6034 (5)	6339 (4)	51 (3)
C(11)	8941 (6)	7229 (5)	7560 (3)	43 (2)
C(12)	9537 (7)	7808 (5)	8114 (4)	64 (3)
C(13)	10095 (8)	8667 (6)	7909 (5)	76 (4)
C(14)	10026 (7)	8954 (5)	7159 (5)	66 (3)
C(15)	9436 (7)	8384 (6)	6604 (5)	75 (3)
C(16)	8912 (7)	7536 (6)	6800 (4)	66 (3)
C(21)	9327 (6)	5164 (5)	7751 (3)	40 (2)
C(22)	8931 (7)	4224 (5)	7776 (4)	53 (3)
C(23)	9792 (7)	3485 (5)	7775 (4)	61 (3)
C(24)	11027 (8)	3701 (6)	7735 (4)	64 (3)
C(25)	11424 (7)	4628 (6)	7696 (4)	64 (3)
C(26)	10557 (7)	5361 (5)	7708 (4)	51 (3)
C(31)	7818 (7)	6174 (5)	8778 (4)	48 (3)
C(32)	8733 (7)	6063 (5)	9369 (4)	56 (3)
C(33)	8469 (8)	6154 (5)	10125 (4)	64 (3)
C(34)	7262 (9)	6348 (6)	10291 (5)	77 (4)
C(35)	6344 (8)	6434 (7)	9707 (5)	85 (4)
C(36)	6622 (7)	6343 (6)	8950 (4)	62 (3)
C(41)	2988 (6)	6032 (4)	5692 (4)	44 (2)
C(42)	3255 (7)	5917 (5)	4940 (4)	57 (3)
C(43)	2351 (8)	5913 (6)	4339 (4)	72 (3)
C(44)	1131 (8)	6000 (7)	4499 (5)	77 (4)
C(45)	838 (8)	6124 (6)	5246 (5)	83 (4)
C(46)	1756 (7)	6141 (6)	5838 (5)	68 (3)
C(51)	7728 (9)	6906 (8)	4183 (5)	94 (5)
C(52)	8086 (9)	7791 (8)	3947 (5)	95 (5)
C(53)	7727 (9)	8577 (7)	4330 (6)	93 (4)
C(54)	7016 (9)	8499 (7)	4943 (5)	91 (4)
C(55)	6666 (9)	7619 (7)	5170 (5)	88 (4)
C(56)	7019 (8)	6808 (7)	4797 (5)	86 (4)

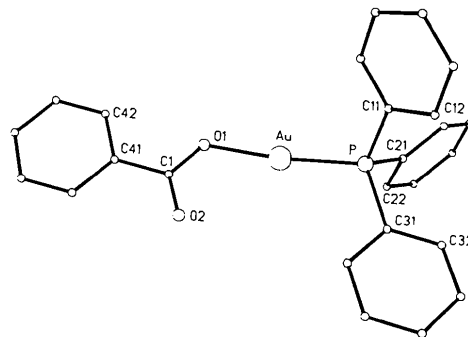


Fig. 1. The benzoato(triphenylphosphine)gold(I) molecule, showing the atom-numbering scheme. (H atoms omitted: arbitrary radii.)

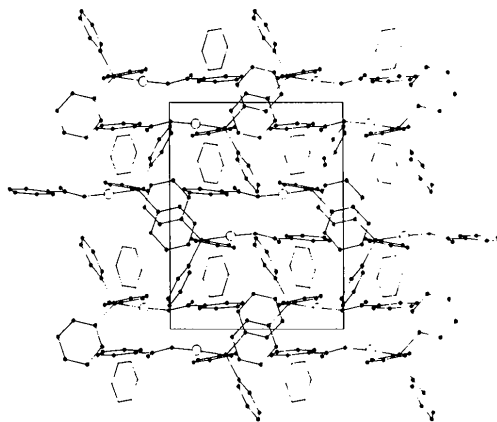


Fig. 2. Packing diagram projected down *c*. Open circles, Au; benzene rings with point atoms; filled circles, all other atoms. H atoms omitted. The apparent stacking of some aromatic rings is an artefact of projection.

The title compound is not isostructural with other Ph₃PAuX derivatives (Jones, 1984); this may be attributed to the bulkier benzoate group and the presence of the benzene of crystallization. The latter is well ordered.

There are no unusually short intermolecular contacts; the benzene occupies holes in the lattice without participation in stacking interactions (Fig. 2).

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Table 2. Bond lengths (Å) and selected bond angles (°)

Au—P	2.213 (3)	Au—O(1)	2.033 (6)
C(1)—O(1)	1.297 (10)	C(1)—O(2)	1.232 (10)
C(1)—C(41)	1.490 (10)	C(11)—P	1.810 (8)
C(11)—C(12)	1.377 (11)	C(11)—C(16)	1.388 (10)
C(12)—C(13)	1.397 (12)	C(13)—C(14)	1.362 (13)
C(14)—C(15)	1.368 (12)	C(15)—C(16)	1.362 (13)
C(21)—P	1.821 (8)	C(21)—C(22)	1.376 (11)
C(21)—C(26)	1.367 (11)	C(22)—C(23)	1.387 (12)
C(23)—C(24)	1.378 (13)	C(24)—C(25)	1.362 (13)
C(25)—C(26)	1.386 (12)	C(31)—P	1.822 (8)
C(31)—C(32)	1.380 (11)	C(31)—C(36)	1.371 (12)
C(32)—C(33)	1.374 (11)	C(33)—C(34)	1.387 (14)
C(34)—C(35)	1.371 (13)	C(35)—C(36)	1.380 (12)
C(41)—C(42)	1.373 (10)	C(41)—C(46)	1.385 (11)
C(42)—C(43)	1.376 (11)	C(43)—C(44)	1.375 (14)
C(44)—C(45)	1.373 (14)	C(45)—C(46)	1.376 (12)
C(51)—C(52)	1.361 (17)	C(51)—C(56)	1.370 (14)
C(52)—C(53)	1.352 (16)	C(53)—C(54)	1.368 (15)
C(54)—C(55)	1.349 (15)	C(55)—C(56)	1.369 (15)
Au...O(2)	3.037 (8)		
P—Au—O(1)	173.7 (2)	Au—P—C(11)	109.9 (3)
Au—P—C(21)	115.0 (3)	C(11)—P—C(21)	106.8 (4)
Au—P—C(31)	113.1 (3)	C(11)—P—C(31)	107.0 (4)
C(21)—P—C(31)	104.4 (4)	Au—O(1)—C(1)	118.0 (5)
O(1)—C(1)—O(2)	123.6 (8)	O(1)—C(1)—C(41)	114.9 (7)
O(2)—C(1)—C(41)	121.5 (8)		