Related literature. The present investigation confirms the essential features of the CdSb structure as determined from photographic data by Almin (1948). The most important difference is the Cd—Cd distance, which is significantly longer than previously found and has the same value [3·136 (1) Å] as the mean Cd—Cd distance in metallic cadmium (Donohue, 1974). This excludes the possibility of substantial covalent interactions between the Cd atoms, in spite of the fact that the Cd atoms can be grouped into pairs in the structure. The Sb—Sb distance [2·810 (1) Å] agrees well with that in other diantimonides (Donaldson, Kjekshus, Nicholson & Rakke, 1975). The description of the CdSb-type structure {also adopted by ZnSb (Almin, 1948) and the high-pressure phases ZnAs and CdAs (Clark & Range, 1975, 1976)} as a heavily distorted diamond structure (Almin, 1948) is rather arbitrary. It should better be viewed as a binary variant of Si-III (Kasper & Richards, 1964), which in turn is an example of a dense sphere packing in space group *Ia*3 (Fischer, 1973). The group–subgroup relations between this sphere packing and the CdSb-type structure have already been discussed (Clark & Range, 1976).

For the stable and metastable phase diagram of the Cd–Sb system see Hansen (1958). Belash & Ponyatovskii (1974) reported a high-pressure decomposition of CdSb into Cd and Sb at 3·5 GPa which is unlikely from the phase diagram and could not be verified in our own high-pressure experiments.

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(Trifluoroacetato)(triphenylphosphine)gold(I)

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Abstract. $[Au(C_2F_3O_2)\{(C_6H_5)_3P\}]$, $M_r = 572{\cdot}27$, orthorhombic, $P2_12_12_1$, $a = 11{\cdot}771\ (2)$, $b = 11{\cdot}906\ (3)$, $c = 14{\cdot}169\ (3)$ Å, $V = 1986{\cdot}0\ (7)$ Å^3, $Z = 4$, $D_x = 1{\cdot}914$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 75{\cdot}12$ cm^{-1}, $F(000) = 1088$. Final $R = 0{\cdot}036$ for 1309 absorption-corrected reflections. Not isostructural with Ph_3AuCl, Ph_3AuBr, and $Ph_3Au(O_2CCH_3)$. The Au—O bond length is 2·107 (9) Å with Au—P equal to 2·208 (4) Å.

Experimental. The title compound was prepared by the reaction of Ph_3PAuCl with AgO_2CCF_3 in anhydrous toluene. Crystals were grown from anhydrous petroleum ether. A colorless crystal 0·30 × 0·2 × 0·2 mm was used in this study. The X-ray data were measured using a Nicolet *R*3*m* diffractometer with Mo *K*α radiation and a graphite monochromator. Cell constants were determined using 25 reflections in the 2θ range 11–22°. A total of 2045 reflections in the 2θ range 3–50° (*h* 0 to 14, *k* 0 to 15, *l* 0 to 17) was measured. Two standard reflections were measured after every 98 reflections and were used to correct small variations (±2·5% or ±1·6σ) in their intensities. The data were corrected for absorption using the ψ-scan

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Table 1. *Final positional* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^3$)

	x	*y*	*z*	U_{eq}*
Au	1916 (1)	6291 (1)	4635 (1)	67 (1)
P	1257 (3)	7901 (3)	5183 (3)	56 (1)
O(1)	2509 (9)	4712 (7)	4179 (7)	78 (4)
C(1)	2251 (15)	3953 (13)	4720 (15)	86 (7)
C(2)	2717 (20)	2808 (14)	4418 (13)	114 (9)
O(2)	1749 (11)	4015 (10)	5462 (10)	122 (6)
F(1)	2190 (32)	1922 (19)	4871 (23)	157 (13)
F(2)	3142 (34)	2706 (21)	3729 (23)	310 (22)
F(3)	3873 (14)	2762 (16)	4646 (16)	131 (8)
F(1′)	1721 (67)	2365 (47)	3912 (54)	346 (43)
F(2′)	2655 (34)	2544 (22)	3571 (19)	151 (16)
F(3′)	2722 (39)	2262 (24)	5160 (22)	115 (18)
C(12)	3175 (8)	9163 (8)	4877 (5)	72 (5)
C(13)	4066	9875	5129	80 (7)
C(14)	4152	10269	6054	93 (8)
C(15)	3348	9950	6726	94 (7)
C(16)	2458	9238	6473	68 (5)
C(11)	2371	8844	5548	57 (5)
C(22)	−416 (8)	8475 (6)	6480 (7)	60 (5)
C(23)	−1091	8279	7272	82 (7)
C(24)	−977	7278	7776	97 (8)
C(25)	−189	6474	7487	96 (7)
C(26)	486	6670	6695	82 (6)
C(21)	373	7671	6191	55 (5)
C(32)	−296 (10)	8091 (8)	3748 (8)	91 (7)
C(33)	−1020	8661	3133	149 (13)
C(34)	−1042	9833	3131	138 (13)
C(35)	−339	10434	3742	115 (9)
C(36)	385	9863	4356	90 (7)
C(31)	407	8691	4359	61 (5)

* Equivalent isotropic *U* defined as one third of the trace of the orthogonalized U_{ij} tensor.

method (transmissions 0·506 to 0·603). The structure was solved by Patterson and Fourier methods. The refinement was by blocked-cascade least-squares methods. The phenyl rings were treated as a rigid body with a C—C distance of 1·395 and a C—H distance of 0·960 Å. The CF_3 group was undergoing large thermal motion which was approximated by six half-fluorine atoms. The weights used were $w = [\sigma^2(F_o) + gF_o^2]^{-1}$ where *g* was refined to 0·000305. The final refinement of 227 parameters and 1309 reflections [$I > 3\sigma(I)$] converged to a final *R* (*F*) of 0·036 and *wR* of 0·033 with a g.o.f. of 1·24. The final difference Fourier synthesis showed $\Delta\rho_{min}$ of −0·53 and $\Delta\rho_{max}$ of 1·5 e $Å^{-3}$ in the vicinity of the Au atom. $(\Delta/\sigma)_{max}$ was 0·12. All calculations were carried out using the *SHELXTL* program (Sheldrick, 1986), on an Eclipse Model 30 computer. The scattering factors used in the *SHELXTL* program are the analytical form given in *International Tables for X-ray Crystallography* (1974). The final atomic coordinates are given in Table 1. Selected bond lengths and angles are given in Table 2.* A view of the molecule is given in Fig. 1.

Table 2. *Selected bond distances* (Å) *and bond angles* (°)

Au—P	2·208 (4)	Au—O(1)	2·107 (8)
P—C(11)	1·802 (10)	P—C(21)	1·789 (10)
P—C(31)	1·802 (12)	O(1)—C(1)	1·223 (20)
C(1)—C(2)	1·530 (24)	C(1)—O(2)	1·208 (25)
P—Au—O(1)	176·9 (3)	Au—P—C(11)	112·7 (3)
Au—P—C(21)	110·6 (3)	C(11)—P—C(21)	106·8 (4)
Au—P—C(31)	114·9 (4)	C(11)—P—C(31)	105·4 (5)
C(21)—P—C(31)	105·9 (5)	Au—O(1)—C(1)	112·7 (11)
O(1)—C(1)—C(2)	113·3 (16)	O(1)—C(1)—O(2)	128·4 (15)
C(2)—C(1)—O(2)	118·2 (16)	P—C(11)—C(12)	117·8 (3)
P—C(11)—C(16)	122·2 (3)	P—C(21)—C(22)	121·1 (3)
P—C(21)—C(26)	118·9 (3)	P—C(31)—C(32)	117·6 (4)
P—C(31)—C(36)	122·3 (4)		

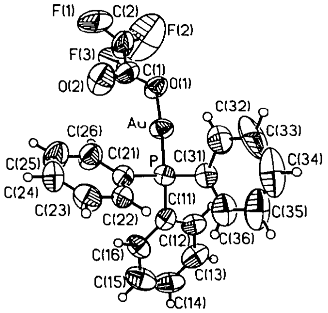

Fig. 1. A view of the (trifluoroacetato)(triphenylphosphine)gold(I) molecule showing the atomic numbering and 50% thermal ellipsoids. Only one set of fluorine atoms of the disordered CF_3 group is shown.

Related literature. The Au—P distances in a series of Ph_3PAuX complexes (Jones, 1981) range from 2·24 to 2·29 Å. The Au—O bond length has been discussed by Jones (1984). Although a number of Ph_3PAuX complexes crystallized with the space group $P2_12_12_1$ and approximately the same cell constants (*e.g.* Baenziger, Bennett & Soboroff, 1976; Einstein & Restivo, 1975; Jones, 1984), Ph_3AuCF_3COO does not appear to be isostructural with them.

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* Lists of distances and angles, anisotropic thermal parameters, H-atom parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51216 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.