significant changes in the *R* indices. Final atomic coordinates and thermal parameters are given in Tables 1 and 2, and the resulting bond lengths and angles in Tables 3 and 4.*

Discussion. Trimethyltin moieties are linked by disordered –O–S(Me)–O– groups to form infinite helical chains along **c**, with approximately trigonal bipyramidal geometry at Sn (Fig. 1). There are two crystallographically independent Me_3Sn groups, each arranged with one of the Sn–C bonds along a crystallographic twofold axis so that the group is exactly planar and the Sn atom is coordinated symmetrically by the O atoms to which it is bonded. Symmetrical bridging is also found in $Me_3SnOS(O)CH_2CCH$ [Ginderow & Huber (1973); Sn–O 2·306 (10) and 2·296 (10) Å] where, however, the chairs adopt a zigzag rather than helical conformation. The Sn–O distances in the methylsulphinate are similar to those in trimethyltin methoxide [2·20 (2) and 2·26 (2) Å; Domingos & Sheldrick (1974)], but shorter than the values quoted above for the $-OS(O)CH_2CCH$ derivative; this, and the relatively short Sn–C bonds, may arise from librational effects. Subsequent inspection of the X-ray photographs revealed the presence of weak diffuse low-order reflexions corresponding to a *P* rather than a *C* lattice, indicating some short-range order in the conformation adopted by the disordered SMe groups.

We are grateful to the Science Research Council for providing the diffractometer and for financial support to RT. The calculations were performed on the Cambridge University IBM 370/165 computer with programs written by GMS. Fig. 1 was drawn with *PLUTO* written by Dr W. D. S. Motherwell.

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31977 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1 NZ, England.

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Methyl(triphenylphosphine)gold

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Abstract. $C_{19}H_{18}AuP$, monoclinic, $P2_1/n$, $a = 17{\cdot}29$ (1), $b = 11{\cdot}27$ (1), $c = 8{\cdot}92$ (1) Å, $\beta = 104{\cdot}5$ (1)°, $U = 1682$ Å^3, $Z = 4$, $D_x = 1{\cdot}88$ g cm^{-3}. There is essentially linear coordination of gold [P–Au–C = 179·1 (8)°] with Au–C 2·124 (28) and Au–P 2·279 (8) Å. The structure was refined to an *R* of 0·092 for 1867 unique diffractometer data.

Introduction. Previous crystallographic studies of Au^I complexes containing Au–C bonds (Bellon, Manassero & Sansoni, 1969; Corfield & Shearer, 1967; Baker & Pauling, 1972) have involved *sp* or sp^2 hydridized C, in which π-bonding between Au^I and C is possible. The Au^I–C(sp^3) distance in the title compound provides a suitable reference bond length in which π-bonding is absent.

Colourless crystals were obtained by recrystallization from benzene/light petroleum of a sample obtained by standard methods (Tamaki & Kochi, 1973), and mounted in Lindemann glass capillary tubes. Intensities were measured on a Stoe automated two-circle diffractometer, with Mo $K\alpha$ radiation ($\lambda = 0{\cdot}71069$ Å) and a graphite crystal monochromator. Cell dimensions were obtained by a least-squares fit to 652 *hk*0 and 444 *h*0*l* diffractometer zero-layer ω-angle measurements. The crystals possessed large mosaic spreads and the data were clearly of mediocre quality; only the 00*l* data (layers *hk*0–10) were used for structure refinement. Lp and empirical absorption corrections were applied. 2580 reflexions were measured; averaging equivalent reflexions gave 1867 reflexions with $I > 3\sigma(I)$ based on counting statistics.

The atoms were located from Patterson and difference syntheses; the structure was refined by blockedcascade least squares with anisotropic temperature factors for Au and P and isotropic C. Since the interlayer scale factors were also refined the values obtained for U_{33} are physically dubious. Rigid phenyl groups were employed (C—H 1·08, C—C 1·395 Å, all angles 120°); the reduction in R when these constraints were removed (0·004 for 36 extra parameters) was not considered to be significant. An overall isotropic temperature factor was employed for the phenyl H atoms; it did not prove possible to locate the methyl H atoms. Complex neutral-atom scattering factors were employed; the weighting scheme was $w = [\sigma^2(F) + 0{\cdot}00035F_o^2]$. The refinement converged to $R' = \Sigma w^{1/2}\Delta/\Sigma w^{1/2}|F_o| = 0{\cdot}097$, and $R = 0{\cdot}092$. Final atomic coordinates and thermal parameters are given in Tables 1 and 2, and the resulting interatomic distances and angles in Tables 3 and 4.* Fig. 1 shows the structure of the molecule.

Table 1. *Atom coordinates* (×10⁴) *and isotropic temperature factors* (Å^2 ×10^3)

	x	y	z	U
Au	1048 (1)	585 (1)	2905 (1)	
P	644 (4)	2305 (5)	1598 (9)	
C(4)	1440 (16)	−1020 (23)	4106 (32)	59 (7)
C(12)	711 (8)	4523 (15)	3124 (22)	64 (7)
C(13)	1126 (8)	5440 (15)	4031 (22)	83 (9)
C(14)	1960 (8)	5435 (15)	4453 (22)	81 (9)
C(15)	2378 (8)	4514 (15)	3968 (22)	92 (10)
C(16)	1963 (8)	3596 (15)	3061 (22)	64 (7)
C(11)	1130 (8)	3601 (15)	2639 (22)	55 (6)
C(22)	717 (11)	1359 (13)	−1223 (23)	66 (7)
C(23)	834 (11)	1382 (13)	−2714 (23)	81 (9)
C(24)	1076 (11)	2429 (13)	−3297 (23)	86 (10)
C(25)	1201 (11)	3453 (13)	−2387 (23)	74 (8)
C(26)	1084 (11)	3429 (13)	−896 (23)	80 (9)
C(21)	841 (11)	2382 (13)	−313 (23)	65 (7)
C(32)	−835 (10)	3262 (15)	−79 (17)	61 (7)
C(33)	−1627 (10)	3601 (15)	−227 (17)	70 (8)
C(34)	−2011 (10)	3295 (15)	918 (17)	74 (8)
C(35)	−1605 (10)	2650 (15)	2212 (17)	71 (8)
C(36)	−813 (10)	2312 (15)	2360 (17)	71 (8)
C(31)	−428 (10)	2618 (15)	1215 (17)	52 (6)
H(22)	529 (11)	548 (13)	−772 (23)	145 (32)
H(23)	737 (11)	590 (13)	−3418 (23)	145 (32)
H(24)	1167 (11)	2448 (13)	−4451 (23)	145 (32)
H(25)	1388 (11)	4263 (13)	−2838 (23)	145 (32)
H(26)	1180 (11)	4221 (13)	−192 (23)	145 (32)
H(12)	66 (8)	4527 (15)	2797 (22)	145 (32)
H(13)	802 (8)	6154 (15)	4406 (22)	145 (32)
H(14)	2281 (8)	6146 (15)	5155 (22)	145 (32)
H(15)	3023 (8)	4510 (15)	4295 (22)	145 (32)
H(16)	2287 (8)	2883 (15)	2686 (22)	145 (32)
H(32)	−537 (10)	3499 (15)	−966 (17)	145 (32)
H(33)	−1942 (10)	4100 (15)	−1299 (17)	145 (32)
H(34)	−2624 (10)	3557 (15)	803 (17)	145 (32)
H(35)	−1902 (10)	2414 (15)	3099 (17)	145 (32)
H(36)	−498 (10)	1813 (15)	3362 (17)	145 (32)

Table 2. *Anisotropic temperature factors* (Å^2 ×10^3)

The temperature factor exponent takes the form: $-2\pi^2(U_{11}h^2a^{*2} + \cdots + 2U_{12}hka^*b^*)$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au	70 (1)	36 (1)	92 (3)	9 (1)	57 (1)	3 (1)
P	66 (4)	37 (3)	80 (5)	4 (3)	54 (4)	−3 (3)

Table 3. *Bond lengths* (Å)

Au—P	2·279 (8)	Au—C(4)	2·124 (28)
P—Au	2·279 (8)	P—C(11)	1·819 (19)
P—C(21)	1·822 (25)	P—C(31)	1·833 (20)
C(4)—Au	2·124 (28)	C(11)—P	1·819 (19)
C(21)—P	1·822 (25)	C(31)—P	1·833 (20)

Discussion. The coordination of Au$^{\rm I}$ is found to be linear within experimental error. The Au—P distance [2·279 (8) Å] is similar to that in Ph_3PAuCN [2·27 (1) Å; Bellon, Manassero & Sansoni (1969)] but longer than in Ph_3PAuCl [2·235 (3) Å; Baenziger, Bennett & Soboroff (1976)]. The Au—C distance [2·124 (28) Å] is significantly longer than the 1·935 (19) Å in (i-$C_3H_7NH_2$)$AuC{\equiv}CC_6H_5$ (Corfield & Shearer, 1967) and 1·85 (4) Å in Ph_3AuCN, even allowing for a shortening of 0·03 Å caused by the change in hybridization of C; this provides evidence of Au—C π-bonding in the acetylide and cyanide complexes. In contrast, IR evidence suggests little Au$^{\rm I}$—C π-bonding in ClAuCO

Table 4. *Bond angles* (°)

P—Au—C(4)	179·1 (8)	Au—P—C(11)	112·3 (7)
Au—P—C(21)	114·4 (7)	C(11)—P—C(21)	105·6 (10)
Au—P—C(31)	115·1 (7)	C(11)—P—C(31)	104·8 (9)
C(21)—P—C(31)	103·5 (9)	P—C(11)—C(12)	123·2 (6)
P—C(11)—C(16)	116·6 (6)	P—C(21)—C(22)	117·8 (6)
P—C(21)—C(26)	122·2 (6)	P—C(31)—C(32)	122·1 (7)
P—C(31)—C(36)	117·5 (7)		

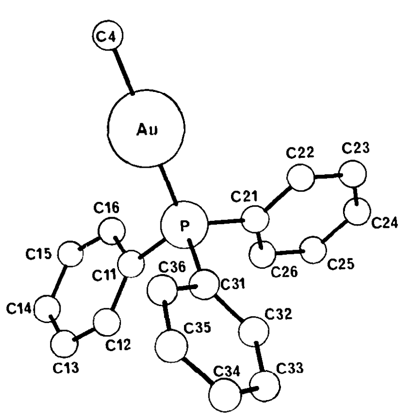

Fig. 1. The methyl(triphenylphosphine)gold molecule.

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(Belli dell'Amico & Calderazzo, 1973). The shortest Au—Au distance in the present compound is 5·68 Å; so there is no evidence of Au—Au interactions as in (i-$C_3H_7NH_2$)$AuC{\equiv}CC_6H_5$ (3·27 and 3·72 Å) and (piperidine)AuCl [3·30 Å; Guy, Jones, Mays & Sheldrick (1977)].

We are grateful to the Science Research Council for providing the diffractometer, and for financial support to PDG and JJG. The calculations were performed with the Cambridge University IBM 370/165 computer and programs written by GMS, and Fig. 1 was drawn with *PLUTO* written by Dr W. D. S. Motherwell.

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Trifluoromethylselenium Trichloride

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Abstract. CF_3SeCl_3, orthorhombic, *Pbca*, $a = 18{\cdot}938$ (23), $b = 7{\cdot}399$ (20), $c = 18{\cdot}880$ (22) Å, $U = 2646$ Å^3, $Z = 16$, $D_x = 2{\cdot}55$ g cm^{-3}, μ(Mo $K\alpha$) = 66·08 cm^{-1}. The structure was solved by direct methods and refined to an R of 0·093 for 474 unique diffractometer data. It consists of discrete dimers $(CF_3SeCl_3)_2$, in which each Se is coordinated by a CF_3 group, two bridging Cl and two terminal Cl in an approximately square-pyramidal arrangement with axial CF_3. The two $SeCl_4$ planes make an angle of 154° with one another, and the dimer possesses approximate *mm* symmetry.

Introduction. Vapour-phase studies on the Group VI tetrahalides are consistent with structures based on a trigonal bipyramid with an equatorial position occupied by a lone pair, in accordance with the VSEPR hypothesis. Similar geometries are found in crystalline Ph_2SeX_2 (McCullough & Hamburger, 1941, 1942) and (p-tolyl)$_2SeX_2$ (McCullough & Marsh, 1950) (X = Cl, Br). On the other hand, the crystal structure of $TeCl_4$ (Buss & Krebs, 1971) contains isolated tetramers in which each Te is surrounded by a distorted octahedron of three terminal and three bridging Cl atoms. The vibrational spectrum of CF_3SeCl_3 also indicates extensive Cl-bridging in the solid, but an X-ray crystallographic study was necessary to determine the structure.

A sample of CF_3SeCl_3 was prepared by the action of excess Cl_2 on $(CF_3Se)_2$ and left in a sealed tube for about a year, during which time a few well formed crystals grew by sublimation. These were transferred to Lindemann glass capillary tubes in a dry bag because the compound is extremely sensitive to moisture. Intensities were determined with an automated Stoe two-circle diffractometer, Mo $K\alpha$ radiation, graphite monochromator and a crystal 0·17 × 0·57 × 0·23 mm (layers $h0$–$8l$). 933 reflexions were measured in an approximately constant count mode; after rejection of reflexions with a net count less than $2{\cdot}5\sigma$ based on counting statistics, equivalent data were merged to give 474 unique reflexions. Lorentz, polarization and absorption corrections were applied. a and c were obtained by a least-squares fit to the diffractometer ω angle measurements of 120 $h0l$ reflexions; b was obtained from diffractometer μ measurements.

The structure was solved by multisolution sigma-2 sign expansion followed by successive difference syntheses. It was apparent that the F atoms of both crystallographically independent CF_3 groups were smeared out by the effects of thermal motion, and in the final full-matrix least-squares cycles it was necessary to constrain C—F to 1·33 Å and F—C—F to 108·5°. Anisotropic temperature factors were employed for the Se and F atoms; interlayer scale factors were fixed at the values to which they had refined during earlier cycles in which only isotropic temperature factors had been used, so the final values of U_{22} have