

## Bis(diphenylmethylphosphine)gold(I) Hexafluorophosphate

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**Abstract.**  $C_{26}H_{26}P_3AuF_6$ , monoclinic,  $C2/c$ ;  $a=23.23$  (2),  $b=10.33$  (1),  $c=15.31$  (2) Å,  $\beta=131.28$  (10)°,  $U=2761$  Å<sup>3</sup>;  $Z=4$ ,  $D_m=1.76$  (floatation),  $D_x=1.786$  g cm<sup>-3</sup>. The structure consists of centrosymmetric  $(Ph_2MeP)_2Au^+$  cations, and  $PF_6^-$  anions which lie on twofold axes and exhibit twofold disorder. The structure was refined to an  $R$  of 0.0483 for 1760 independent observed reflexions.

**Introduction.** The structure of  $(Ph_2MeP)_2Au^+PF_6^-$  has been determined as part of a study of gold compounds. Many compounds are known which contain ions of the form  $L_2Au^+$  or  $LAuL'^+$  (e.g. Westland, 1969; Bonati & Minghetti, 1973), but no crystal structure determinations have been reported.

Colourless crystals were obtained from dichloromethane/ether and were stable to air and X-rays. Intensities were determined with a Syntex  $P2_1$  four-circle diffractometer, Mo  $K\alpha$  radiation, a graphite monochromator and a crystal  $0.06 \times 0.2 \times 0.4$  mm. 5111 reflexions were measured; averaging equivalent reflexions gave 1760 unique data with  $F > 4\sigma(F)$  based on counting statistics.

The non-hydrogen atoms were located from Patterson and difference syntheses; the Au and P (of  $PF_6^-$ ) atoms occupy special positions (0,0,0) and (0, $y$ , $\frac{1}{4}$ ) respectively. Rigid phenyl groups with C-C 1.395, C-H 1.08 Å and all angles 120° were employed

in the final refinement because the reduction in  $R'$  (0.0017 for 24 additional parameters), when the C atoms were allowed to refine freely, was not considered to be significant. A rigid methyl group was employed with C-H 1.08 Å and H-C-H 109.5°. Separate overall isotropic temperature factors were employed for the

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

	$x$	$y$	$z$	$U$
Au(1)	0	0	0	
P(1)	688 (1)	1742 (2)	148 (2)	
P(2)	0	6440 (4)	-2500	
F(1)	307 (11)	5768 (18)	-1328 (16)	121 (5)
F(2)	360 (11)	5394 (17)	-2812 (17)	109 (5)
F(3)	-794 (12)	5815 (23)	-3250 (19)	150 (6)
F(4)	-227 (12)	7657 (17)	-2116 (17)	123 (6)
F(5)	875 (11)	7162 (17)	-1673 (16)	124 (5)
F(6)	-147 (10)	7283 (16)	-3491 (16)	110 (5)
C(11)	982 (4)	1583 (5)	-684 (6)	50 (2)
C(12)	960 (4)	384 (5)	-1125 (6)	64 (3)
C(13)	1237 (4)	262 (5)	-1699 (6)	82 (3)
C(14)	1536 (4)	1339 (5)	-1831 (6)	83 (3)
C(15)	1558 (4)	2538 (5)	-1390 (6)	87 (3)
C(16)	1280 (4)	2659 (5)	-817 (6)	60 (3)
C(21)	1574 (4)	1981 (6)	1630 (6)	57 (2)
C(22)	2192 (4)	1157 (6)	2088 (6)	81 (3)
C(23)	2867 (4)	1291 (6)	3242 (6)	109 (4)
C(24)	2925 (4)	2249 (6)	3939 (6)	107 (4)
C(25)	2308 (4)	3073 (6)	3481 (6)	105 (4)
C(26)	1638 (4)	2939 (6)	2327 (6)	79 (3)
H(12)	728	-450	-1023	146 (15)
H(13)	1220	-666	-2040	146 (15)
H(14)	1750	1245	-2275	146 (15)
H(15)	1789	3371	-1493	146 (15)
H(16)	1297	3587	-475	146 (15)
H(22)	2147	415	1548	146 (15)
H(23)	3346	653	3597	146 (15)
H(24)	3448	2353	4833	146 (15)
H(25)	2353	3815	4021	146 (15)
H(26)	1155	3577	1972	146 (15)
C(3)	156 (6)	3242 (10)	-308 (9)	65 (3)
H(31)	-66	3462	112	81 (18)
H(32)	-316	3084	-1225	81 (18)
H(33)	499	4042	-194	81 (18)

Anisotropic temperature factors ( $\text{Å}^2 \times 10^3$ )

The anisotropic temperature factor takes the form:

$$\exp[-2\pi^2(U_{11}h^2a^{*2} + \dots + 2U_{12}hka^*b^*)].$$

	$U_{11}$	$U_{22}$	$U_{33}$	$U_{23}$	$U_{13}$	$U_{12}$
Au(1)	54 (1)	54 (1)	57 (1)	1 (1)	37 (1)	-12 (1)
P(1)	52 (2)	46 (2)	49 (2)	1 (2)	33 (2)	-7 (2)
P(2)	112 (4)	64 (3)	75 (3)	0	72 (3)	0

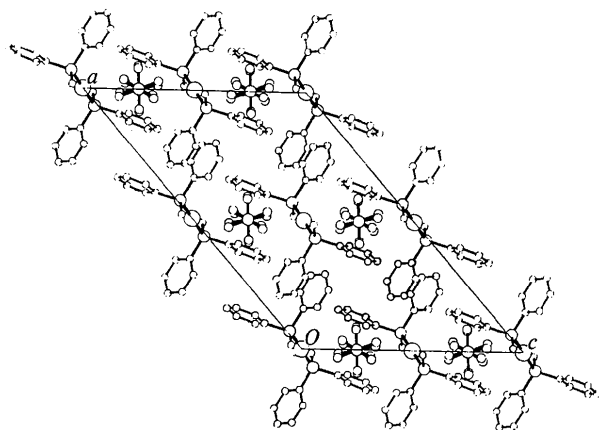


Fig. 1. The structure in projection down  $y$ , showing both positions of the disordered  $PF_6^-$  ion (H atoms omitted for clarity).

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

Au(1)—P(1)	2.316 (4)	C(11)—P(1)	1.808 (8)
C(21)—P(1)	1.812 (8)	C(3)—P(1)	1.810 (8)
P(2)—F(1)	1.588 (20)	P(2)—F(2)	1.618 (20)
P(2)—F(3)	1.531 (24)	P(2)—F(4)	1.617 (19)
P(2)—F(5)	1.702 (21)	P(2)—F(6)	1.579 (18)
C(11)—P(1)—Au(1)	114.6 (4)	C(21)—P(1)—Au(1)	111.7 (4)
C(21)—P(1)—C(11)	104.4 (5)	C(3)—P(1)—Au(1)	112.1 (5)
C(3)—P(1)—C(11)	106.6 (6)	C(3)—P(1)—C(21)	106.9 (6)
C(12)—C(11)—P(1)	120.8 (4)	C(16)—C(11)—P(1)	119.0 (4)
C(22)—C(21)—P(1)	119.3 (4)	C(26)—C(21)—P(1)	120.7 (4)
H(31)—C(3)—P(1)	115.0	H(32)—C(3)—P(1)	102.8
H(33)—C(3)—P(1)	110.4		
F(1)—P(2)—F(2)	96.2 (11)	F(1)—P(2)—F(3)	94.8 (12)
F(1)—P(2)—F(4)	86.6 (11)	F(1)—P(2)—F(5)	85.7 (11)
F(1)—P(2)—F(6)	168.0 (12)	F(2)—P(2)—F(3)	95.7 (12)
F(2)—P(2)—F(4)	169.2 (11)	F(2)—P(2)—F(5)	85.2 (11)
F(2)—P(2)—F(6)	84.9 (11)	F(3)—P(2)—F(4)	94.6 (12)
F(3)—P(2)—F(5)	178.9 (14)	F(3)—P(2)—F(6)	97.0 (13)
F(4)—P(2)—F(5)	84.6 (11)	F(4)—P(2)—F(6)	90.3 (11)
F(5)—P(2)—F(6)	82.4 (11)		

phenyl and methyl H atoms. The  $\text{PF}_6^-$  ion is disordered, the ion occupying either of two positions related by a twofold axis (both positions are shown in Fig. 1). The F atoms all have a site occupation factor of 0.5. The structure was refined (with complex neutral atom scattering factors) to  $R' = \sum w^{1/2} \Delta / \sum w^{1/2} |F_o| = 0.0518$ ; the corresponding unweighted  $R$  was 0.0483. The weighting scheme was  $w = 1/[\sigma^2(F) + 0.001F^2]$ .\*

Final atomic coordinates and thermal parameters are given in Table 1 and interatomic distances and angles in Table 2.

\* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31721 (12 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

We also succeeded in refining the structure, without  $\text{PF}_6^-$  disorder, in the space group  $Cc$  (the alternative space group consistent with the systematic absences). The enantiomorphs converged to  $R = 0.0461$  and 0.0465. In view of the large number of extra parameters (45), large standard deviations and the chemically less reasonable dimensions (especially for the  $\text{PF}_6^-$  ion) which resulted, we prefer the disordered centrosymmetric model. It is unlikely that X-ray diffraction alone could distinguish between the two models.

**Discussion.** The P—Au—P angle in  $(\text{Ph}_2\text{MeP})_2\text{Au}^+$  is exactly  $180^\circ$ , since the Au atom lies on a special position at a centre of symmetry. Linear coordination is generally found for  $\text{Au}^I$  ( $d^{10}$ ), e.g. in  $\text{Ph}_3\text{PAuCl}$  the P—Au—Cl angle is  $179.63(8)^\circ$  (Baenziger, Bennett & Soboroff, 1976). Thus the  $\text{L}_2\text{Au}^+$  cation has, as would be expected, essentially the same coordination geometry as uncharged  $\text{Au}^I$  complexes. The Au—P distance (2.316 Å) is rather greater than in  $\text{Ph}_3\text{PAuCl}$  (2.235 Å).

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