The Molecular Structure of Chlorobis(pentafluorophenyl)triphenylphosphinegold(III)

By R. W. BAKER* and PETER PAULING

(*William Ramsay and Ralph Forster Laboratories, University College, Gower Street, London, W.C.*1)

STIMULATED by recent interest in gold complexes containing fluorinated ligands,[1] we have analysed the crystal structure of chlorobis(pentafluorophenyl)triphenylphosphinegold(III) prepared in this laboratory by Dr. P. Royo. Crystals of $Cl(C_6F_5)_2PPh_3Au^{III}$ are prisms with badly developed domes, of the tetragonal system, Laue group $4/mmm$, space group $P4_2bc$, $a = b = 2556 \pm 1$ pm., $c = 906{\cdot}9 \pm 0{\cdot}3$ pm., $Z = 8$, $D_c = 1776$ kg. m.$^{-3}$, D_m between 1250 and 2270 kg. m.$^{-3}$ (an exact density was not determined). Three dimensional X-ray diffraction data were collected on a computer-controlled Stoe four-circle diffractometer using Mo-K_α radiation. 3676 diffraction maxima in the range $2\theta = 1°$—35° were measured resulting in 711 independent observations ($I_{obs} \geqslant 3\sigma(I)$). The structure was solved by Patterson and Fourier methods and refined by least-squares analysis to $R = 0{\cdot}068$. The isotropic thermal parameters of all the light atoms are high (average B is 0·08 nm.^{2} for carbon and 0·1 nm.^{2} for fluorine) and the standard deviations of the positions of light atoms are about 8 pm.

As seen in the Figure, the gold atom is four-co-ordinated with ligands at the vertices of a square, the two pentafluorophenyl groups being *cis* to each other. The gold, chlorine, phosphorus and two co-ordinating carbon atoms lie in a single plane to within experimental error. With respect to the crystallographic axes the direction cosines of the plane normal (all atoms weighted equally) are 0·3218, −0·5968, and 0·7350, the position of the centroid is 576, 79, and 4 pm., and the deviations from the plane are Au −3, Cl +15, P −13, C(19) +15, and C(30) −14 pm.

The angles between the planes of the two pentafluorophenyl groups and the co-ordination plane are equal to within experimental error, being 77° for the ring bonded through C(19), and 76° for the ring bonded through C(30). Bond distances and angles for the co-ordinating atoms are given in the Table.

The Au–Cl, Au–P, and Au–C bond distances may be compared with those found in related compounds which are also given in the Table. Standard deviations of some distances are not quoted, but in general the differences are not significant. The difference between the Au–Cl distance in this compound and the Au–non-bridging Cl distances of 223 and 225 ± 2 pm. in $Cl_6Au_2^{III}$ [2] is seven times the estimated standard deviations of these distances and this difference presumably is significant. Structure analyses of compounds with gold–aryl bonding have not been reported in the literature up to the beginning of 1969 and we cannot compare the gold–carbon distances with those of other structures.

Bond distances and angles of the co-ordination sphere of $Cl(Ph_3P)(C_6F_5)_2Au^{III}$ *and those reported for related compounds*

Au–Cl	238 ± 2 pm.	223 ± 2 pm. 225 ± 2	} in $Cl_6Au_2^{III}$ [2]
Au–P	237 ± 3	250	in $Br_3(Ph_3P)Au^{III}$ [3]
Au–C(19)	212 ± 9	212 ±14	in $K[(CN)_2Au^{I}]$[4]
Au–C(30)	218 ± 10		
P–Au–Cl	91 ± 1°		
P–Au–C(19)	90 ± 2		
P–Au–C(30)	179 ± 3		
Cl–Au–C(19)	174 ± 2		
Cl–Au–C(30)	88 ± 3		
C(19)–Au–C(30)	91 ± 3		

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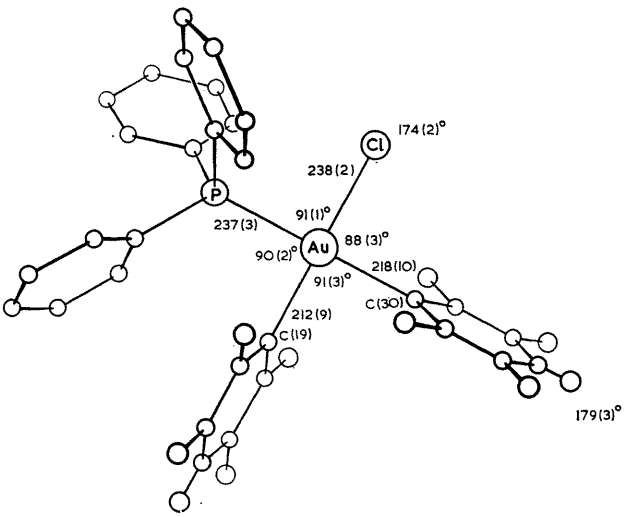

FIGURE. *Molecular structure of chlorobis(pentafluorophenyl) triphenylphosphinegold*(III).

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