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Chloro(triphenylphosphine)gold(I)

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Abstract. Chloro(triphenylphosphine)gold(I), $(C_6H_5)_3PAuCl$, prepared by reacting triphenylphosphine with chloroauric acid in alcohol, crystallizes in the orthorhombic space group $P2_12_12_1$ with $a=12{\cdot}300$ (4), $b=13{\cdot}084$ (4), and $c=10{\cdot}170$ (3) Å; $D_c=1{\cdot}991$, $D_m=1{\cdot}97$ g cm^{-3}, $Z=4$, $R_2=0{\cdot}037$ based on 2109 reflections collected on a four-circle automated diffractometer. The molecule is linear with the gold–phosphorus distance equal to 2·235 (3) Å and the gold–chlorine distance equal to 2·279 (3) Å.

Introduction. Intensity measurements were made from a crystal, $0{\cdot}66(a)\times0{\cdot}41(b)\times0{\cdot}31(c)$ mm, with a four-circle diffractometer (Picker), graphite monochromator, Mo $K\alpha$, $\theta/2\theta$ scan, background measurements at beginning and end of scan, 8898 reflections (total of $\sin\theta/\lambda=0{\cdot}59$), independent reflections = 2109, present independent reflections, 1987. Absorption correction, $\mu=93{\cdot}6$ cm^{-1}, method of Alberti & Gottardi (1966), ranged from 0·054 to 0·115. The structure was solved by Patterson methods, and refined by full-matrix least-squares methods. Hydrogen atoms could not be located from a difference map when $R_2=0{\cdot}075$, so they were placed 1·0 Å from the carbon atoms with C–C–H angles of 120°.

Anisotropic temperature refinement did not yield lower R values until the enantiomorphic coordinates were used. Refinement then quickly led to the final R_1 of 0·031 and $R_2=0{\cdot}037$. Hydrogen atom positions were not refined and the resultant C–H distances ranged from 0·97 to 1·28 Å. Atom scattering factors were taken from *International Tables for X-ray Crystallography* (1962). Dispersion corrections were made for Au, P and Cl. Positional parameters are given in Table 1 and anisotropic B values are given in Table 2. Interatomic distances and angles are given in Table 3.*

Table 1. *Positional parameters for symmetrically unique atoms in chloro(triphenylphosphine)gold*(I)

Hydrogen atoms are designated by the same number as the carbon atom to which they are bonded. No standard deviations appear for hydrogen atoms since they were held at fixed positions during the refinement. The atom parameters are all multiplied by 10^4.

	x	*y*	*z*
Au	695·1 (4)	2404·2 (3)	−1628·2 (4)
Cl	123 (3)	1995 (3)	−3692 (3)
P	1263 (3)	2800 (2)	394 (3)
C(1)	2075 (11)	1832 (11)	1177 (12)
C(2)	2112 (12)	1734 (11)	2509 (13)
C(3)	2796 (15)	986 (13)	3072 (14)
C(4)	3447 (17)	373 (15)	2355 (22)
C(5)	3442 (13)	463 (11)	913 (20)
C(6)	2708 (12)	1196 (11)	391 (15)
C(7)	139 (10)	3003 (10)	1586 (13)
C(8)	8 (11)	3899 (10)	2260 (15)
C(9)	−844 (11)	3927 (11)	3114 (13)
C(10)	−1533 (12)	3093 (14)	3238 (14)
C(11)	−1421 (12)	2220 (12)	2546 (13)
C(12)	−556 (10)	2150 (9)	1724 (14)
C(13)	2046 (10)	3951 (9)	427 (13)
C(14)	1709 (12)	4760 (11)	−392 (17)
C(15)	2359 (13)	5664 (12)	−390 (19)
C(16)	3317 (13)	5728 (10)	315 (15)
C(17)	3637 (13)	4935 (11)	1038 (16)
C(18)	3035 (12)	4028 (10)	1102 (15)
H(2)	1608	2145	3073
H(3)	2910	921	4049
H(4)	3925	−170	2632
H(5)	3921	7	363
H(6)	2662	1264	−610
H(8)	442	4498	2058
H(9)	−1006	4558	3685
H(10)	−2191	3335	3864
H(11)	−1884	1602	2667
H(12)	−471	1509	1180
H(14)	998	4719	−827
H(15)	2095	6307	−901
H(16)	3735	6356	186
H(17)	4368	4966	157
H(18)	3334	3441	1624

Discussion. The molecule of chloro(triphenylphosphine)gold(I) is linear with a P–Au–Cl angle of 179·68 (8)°. The gold–phosphorus distance of 2·235 (3) Å compares favorably with the Au–P distances in $Au_9[P(C_6H_4PCH_3)_3]_8[PF_6]_3$ of 2·23 (2) (Bellon, Cariati, Manassero, Naldini & Sansoni, 1971) and $(C_6H_6)_3PAuCo(CO)_4$ of 2·23 (3) Å (Blundell & Powell, 1971) but it is shorter than the distance in the very similar crystal of $(C_6H_5)_3PAuCN$ of 2·27 (1) Å (Bellon, Manaserro & Sansoni, 1969). The gold–chlorine distance of 2·279 (3) Å is shorter than the covalent radii sum (0·99 + 1·34 Å) for tetrahedral coordination as might be expected from the greater *s* character of the bond. The distance is also much shorter than the Au–Cl distance in bis(triphenylphosphine)gold(I) chloride [2·500 (4) Å] (Baenziger, Dittemore & Doyle, 1974).

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31459 (13 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 2. *Temperature factors for symmetrically unique atoms in chloro(triphenylphosphine)gold*(I)

B_{ij} is defined such that the temperature factor = exp $[-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}kl + B_{23}hl)]$. B for all hydrogen atoms = 5·5. B_{ij} is multiplied $\times 10^4$.

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Au	60·6 (4)	53·9 (3)	79·7 (4)	−8·9 (6)	−14·6 (7)	−3·6 (8)
Cl	93 (3)	88 (3)	86 (4)	−32 (4)	−48 (5)	−13 (5)
P	56 (2)	59 (3)	88 (3)	9 (3)	−7 (4)	7 (5)
C(1)	83 (13)	52 (10)	95 (15)	4 (17)	−44 (22)	5 (19)
C(2)	105 (14)	65 (11)	99 (17)	25 (19)	−29 (24)	32 (22)
C(3)	149 (18)	89 (13)	75 (18)	26 (25)	−43 (27)	10 (25)
C(4)	149 (23)	77 (14)	212 (29)	−40 (26)	−104 (44)	59 (87)
C(5)	80 (16)	44 (12)	207 (29)	34 (17)	31 (31)	75 (28)
C(6)	77 (13)	54 (11)	123 (19)	−21 (17)	35 (25)	31 (23)
C(7)	71 (11)	99 (11)	67 (12)	40 (17)	32 (32)	5 (24)
C(8)	59 (11)	86 (11)	124 (17)	43 (17)	−35 (24)	−59 (26)
C(9)	59 (12)	108 (12)	102 (17)	4 (20)	11 (23)	−64 (24)
C(10)	92 (14)	138 (14)	72 (15)	11 (23)	−14 (25)	−8 (21)
C(11)	86 (13)	117 (15)	89 (15)	−7 (22)	1 (23)	36 (28)
C(12)	52 (11)	86 (10)	124 (15)	−26 (16)	19 (25)	−5 (24)
C(13)	68 (12)	118 (10)	85 (14)	26 (15)	34 (21)	−8 (18)
C(14)	87 (13)	53 (11)	177 (22)	−6 (18)	30 (29)	8 (27)
C(15)	91 (15)	84 (14)	201 (26)	−24 (21)	24 (33)	76 (33)
C(16)	98 (14)	52 (11)	136 (20)	−27 (16)	1 (27)	−41 (25)
C(17)	91 (14)	60 (12)	137 (20)	−4 (20)	−8 (27)	7 (26)
C(18)	84 (19)	64 (11)	133 (19)	−1 (17)	−99 (26)	−22 (23)

Table 3. *Intramolecular bond distances* (Å) *and angles* (°) *in chloro(triphenylphosphine)gold*(I)

Au–P	2·235 (3)		P–C(1)	1·803 (13)		
Au–Cl	2·279 (3)		P–C(7)	1·866 (12)		
			P–C(13)	1·792 (13)		
C(1)–C(2)	1·361 (18)	C(7)—C(8)	1·368 (16)	C(13)–C(14)	1·410 (18)	
C(1)–C(6)	1·396 (19)	C(7)—C(12)	1·417 (17)	C(13)–C(18)	1·409 (19)	
C(2)–C(3)	1·416 (20)	C(8)—C(9)	1·368 (18)	C(14)–C(15)	1·431 (20)	
C(5)–C(6)	1·425 (21)	C(4)—C(12)	1·363 (18)	C(17)–C(18)	1·403 (19)	
C(3)–C(4)	1·352 (24)	C(9)—C(10)	1·392 (19)	C(15)–C(16)	1·390 (21)	
C(4)–C(5)	1·471 (24)	C(10)–C(11)	1·349 (18)	C(16)–C(17)	1·332 (19)	
P—Au–Cl	179·63 (8)		C(1)–P–C(7)	103·3 (4)		
Au–P—C(1)	114·8 (5)		C(1)–P–C(13)	106·2 (5)		
Au–P—C(7)	113·3 (5)		C(7)–P–C(13)	105·8 (4)		
Au–P—C(13)	112·5 (5)					
P——C(1)–C(2)	121·6 (1·3)	P——C(7)—C(8)	122·4 (1·1)	P——C(13)–C(14)	117·4 (1·0)	
P——C(1)–C(6)	118·7 (1·0)	P——C(7)—C(12)	114·0 (1·0)	P——C(13)–C(18)	122·8 (1·1)	
C(6)–C(1)–C(2)	119·7 (1·4)	C(12)–C(7)—C(8)	123·6 (1·1)	C(18)–C(13)–C(14)	118·7 (1·2)	
	360·0		360·0		358·9	
C(1)–C(2)–C(3)	119·2 (1·5)	C(7)—C(8)—C(9)	115·6 (1·5)	C(13)–C(14)–C(15)	117·8 (1·4)	
C(1)–C(6)–C(5)	123·2 (1·4)	C(7)—C(12)–C(11)	119·1 (1·1)	C(13)–C(18)–C(12)	120·2 (1·2)	
C(2)–C(3)–C(4)	123·4 (1·5)	C(8)—C(9)—C(10)	120·7 (1·3)	C(14)–C(15)–C(16)	121·5 (1·5)	
C(6)–C(5)–C(4)	115·3 (1·6)	C(12)–C(11)–C(10)	117·2 (1·4)	C(18)–C(17)–C(16)	121·4 (1·4)	
C(3)–C(4)–C(5)	119·2 (1·9)	C(9)—C(10)–C(11)	123·6 (1·1)	C(15)–C(16)–C(17)	120·0 (1·3)	

In the latter compound roughly trigonal planar coordination leads to reduced *s* character of the bond; in addition, steric interactions with the triphenylphosphine groups also lengthen the bond.

References

ALBERTI, A. & GOTTARDI, G. (1966). *Acta Cryst.* **21**, 833–834.

BAENZIGER, N. C., DITTEMORE, K. M. & DOYLE, J. R. (1974). *Inorg. Chem.* **13**, 803.

BELLON, P. L., CARIATI, F., MANASSERO, M., NALDINI, L. & SANSONI, M. (1971). *Chem. Commun.* p. 1423.

BELLON, P. L., MANASSERO, M. & SANSONI, M. (1969). *Ric. Sci.* **39**, 173.

BLUNDELL, T. & POWELL, H. M. (1971). *J. Chem. Soc.* (*A*), p. 1685.

International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.