SHORT-FORMAT PAPERS

Structure of Chlorobis(dicyclohexylphenylphosphine)gold(I)

By Mariel M. Muir, Sandra I. Cuadrado, James A. Muir and Charles L. Barnes

Departments of Chemistry and Physics, University of Puerto Rico, Rio Piedras, PR 00931, USA

Abstract. $[AuCl\{(C_6H_{11})_2(C_6H_5)P\}_2]$, $M_r = 781\cdot2$, monoclinic, $P2_1$, $a = 11\cdot117$ (4), $b = 13\cdot606$ (5), $c = 12\cdot284$ (4) Å, $\beta = 109\cdot59$ (3)°, $V = 1753$ (2) Å^3, $Z = 2$, $D_x = 1\cdot48$ g cm^{-3}, λ(Mo $K\alpha) = 0\cdot71073$ Å, $\mu = 43\cdot8$ cm^{-1}, $F(000) = 792$, $T = 296$ K, final $R = 0\cdot024$ for 3239 unique observed reflections. The formation of complexes of the type L_nAuX, where L is a phosphine, and X is halide or pseudohalide, shows considerable dependence on the nature of the phosphine. When $L = Ph_3P$, three- and four-coordinated complexes are very easily prepared. However, for $L = Cy_3P$, only linearly coordinated complexes could be isolated. The geometry of the title complex, with $L = Cy_2PhP$, is best described as distorted trigonal planar. The P—Au—P angle is $158\cdot24$ (5)° while the P—Au—Cl angles are $92\cdot63$ (6) and $108\cdot71$ (6)°. Au—P distances are $2\cdot300$ (1) and $2\cdot324$ (1) Å while Au—Cl is $2\cdot744$ (2) Å.

Experimental. The complex Cy$_2$PhPAuCl (0·77 mmol) (Sutton, McGusty, Walz & DiMartino, 1972) was placed in a beaker containing 25 ml ethanol. A sixfold excess of Cy$_2$PhP (3·50 mmol) was added inside a glove bag purged with nitrogen due to the air sensitivity of the phosphine. The beaker was removed from the glove bag after stirring for about 25 min. The expected product is not air sensitive. A gel remained after the ethanol evaporated on standing. Acetone was added and a white powder formed, which was isolated by vacuum filtration and then was dissolved in ethanol. The ethanol solution was evaporated slowly to yield colorless crystals. The product was shown to be chlorobis(dicyclohexylphenylphosphine)gold(I). Analysis: calc. for $C_{36}H_{54}P_2AuCl$: C, 55·35; H, 6·97%; found: C, 55·46; H, 7·01%.

Rectangular plate, D_m not determined, 0·40 × 0·30 × 0·30 mm, Enraf–Nonius CAD-4 diffractometer, monochromated Mo $K\alpha$, ω–θ scan, scan width $0\cdot9 + 0\cdot34\tan\theta°$, $2\theta_{max} = 53°$, lattice parameters from least-squares fit of 24 reflections in the range $10 < \theta < 13°$. Systematic absences $0k0$ ($k = 2n + 1$);

$+h+k\pm l$ with $h \leq 13$, $k \leq 17$, $|l| \leq 15$; three standard reflections, intensities constant within experimental error; total unique reflections measured 3756, 3239 with $F^2 > 2\sigma^2(F_o)$, $\sigma(F_o) = \{[\sigma^2(I_{raw}) + (0\cdot04F_o^2)^2]^{1/2}/2F_o\}$. Absorption corrections from ψ scans, relative transmission factors 0·831 to 0·995. Structure was solved with the Enraf–Nonius *Structure Determination Package* (Frenz, 1986), heavy-atom and difference-Fourier methods; isotropic then anisotropic refinement on F of all non-hydrogen atoms, H atoms at calculated positions [C—H 0·95 Å, U(H)1·3U(C)]; 360 parameters refined, $R = 0\cdot024$, $wR = 0\cdot028$, $w = 1/[\sigma^2(F_o)]$, $S = 1\cdot1$; difference syntheses showed no densities above 0·92 e Å^{-3} (min. −0·22 e Å^{-3}); max. $\Delta/\sigma = 0\cdot01$. Neutral-atom scattering factors were used (*International Tables for X-ray Crystallography*, 1974), and were corrected for anomalous dispersion (Cromer & Liberman, 1970). No correction for secondary extinction.

The atomic coordinates and equivalent isotropic temperature factors are listed in Table 1, and selected bond lengths and angles in Table 2.* An *ORTEP* plot (Johnson, 1976) of the title compound with the atom numbering is shown in Fig. 1, and the packing of the molecules (Motherwell, 1976) in Fig. 2.

Related literature. The structures of other three-coordinated Au^1 complexes have been reported (Baenziger, Dittemore & Doyle, 1974; Clegg, 1978; Muir, Muir & Arias, 1982; Schmidbaur, Wohlleben, Schubert, Frank & Huttner, 1977). The coordination number of Au^1 in this type of complex seems to depend on the cone angle of the phosphine [Cy$_3$P, 170°, linear;

Table 1. *Atomic coordinates and equivalent isotropic temperature factors* (Å^2)

	x	y	z	B(Å^2)
Au	0·19899 (2)	0·250	0·33556 (2)	3·096 (3)
Cl	0·4315 (2)	0·1680 (2)	0·4546 (2)	8·36 (7)
P(1)	0·2541 (1)	0·3996 (1)	0·4305 (1)	2·51 (3)
P(2)	0·0820 (1)	0·1388 (1)	0·2004 (1)	2·73 (3)
C(1)	0·3397 (5)	0·4787 (5)	0·3603 (5)	3·0 (1)
C(2)	0·2529 (6)	0·5031 (7)	0·2376 (6)	5·1 (2)
C(3)	0·3214 (8)	0·561 (1)	0·1701 (6)	8·1 (3)
C(4)	0·4425 (7)	0·513 (1)	0·1707 (7)	7·4 (3)
C(5)	0·5279 (7)	0·4896 (8)	0·2884 (7)	6·2 (2)
C(6)	0·4619 (6)	0·4277 (7)	0·3577 (6)	4·8 (2)
C(7)	0·1160 (5)	0·4717 (5)	0·4328 (4)	3·1 (1)
C(8)	0·1215 (7)	0·5720 (5)	0·4496 (6)	4·2 (2)
C(9)	0·0098 (8)	0·6216 (6)	0·4521 (6)	5·8 (2)
C(10)	−0·0996 (7)	0·5695 (7)	0·4396 (6)	5·7 (2)
C(11)	−0·1037 (6)	0·4716 (7)	0·4224 (6)	5·4 (2)
C(12)	0·0023 (6)	0·4223 (6)	0·4184 (5)	4·0 (1)
C(13)	0·3528 (5)	0·3866 (5)	0·5838 (5)	2·8 (1)
C(14)	0·2878 (9)	0·3169 (7)	0·6410 (6)	7·3 (2)
C(15)	0·372 (1)	0·2981 (8)	0·7698 (7)	9·0 (3)
C(16)	0·4059 (8)	0·3917 (9)	0·8307 (6)	6·6 (2)
C(17)	0·4705 (8)	0·4604 (8)	0·7759 (6)	6·5 (2)
C(18)	0·3901 (7)	0·4796 (6)	0·6489 (6)	4·8 (2)
C(19)	0·0816 (6)	0·0104 (5)	0·2496 (5)	3·2 (1)
C(20)	−0·0122 (7)	−0·0581 (5)	0·1659 (7)	4·6 (2)
C(21)	−0·0046 (8)	−0·1615 (6)	0·2134 (8)	5·9 (2)
C(22)	0·1277 (7)	−0·2018 (6)	0·2538 (6)	5·2 (2)
C(23)	0·2200 (8)	−0·1352 (7)	0·3366 (6)	5·5 (2)
C(24)	0·2121 (8)	−0·0315 (6)	0·2917 (7)	5·1 (2)
C(25)	0·1396 (5)	0·1293 (5)	0·0783 (5)	3·1 (1)
C(26)	0·2679 (6)	0·1493 (6)	0·0971 (6)	4·1 (2)
C(27)	0·3172 (6)	0·1382 (7)	0·0060 (6)	5·3 (2)
C(28)	0·2423 (7)	0·0977 (6)	−0·0965 (6)	4·8 (2)
C(29)	0·1152 (6)	0·0771 (6)	−0·1156 (5)	4·1 (1)
C(30)	0·0653 (6)	0·0910 (5)	−0·0272 (5)	3·6 (1)
C(31)	−0·0852 (6)	0·1761 (5)	0·1379 (5)	3·2 (1)
C(32)	−0·1526 (6)	0·1718 (6)	0·2288 (6)	4·0 (1)
C(33)	−0·2924 (7)	0·2049 (7)	0·1773 (7)	5·9 (2)
C(34)	−0·2998 (7)	0·3075 (7)	0·1257 (7)	5·6 (2)
C(35)	−0·2354 (7)	0·3094 (6)	0·0352 (6)	5·2 (2)
C(36)	−0·0974 (6)	0·2785 (4)	0·0857 (5)	3·7 (1)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as $\frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

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

Au–Cl	2·744 (2)	P(2)–C(19)	1·849 (6)
Au–P(1)	2·324 (1)	P(2)–C(25)	1·822 (7)
Au–P(2)	2·300 (1)	P(2)–C(31)	1·830 (6)
P(1)–C(1)	1·832 (7)	C–C (Cy, ave.)	1·511 (3)
P(1)–C(7)	1·830 (7)	C–C (Ph, ave.)	1·384 (4)
P(1)–C(13)	1·842 (5)		
Cl–Au–P(1)	92·63 (6)	P(1)–C(1)–C(2)	109·7 (4)
Cl–Au–P(2)	108·71 (6)	P(1)–C(1)–C(6)	110·3 (5)
P(1)–Au–P(2)	158·24 (5)	P(1)–C(7)–C(8)	122·5 (5)
Au–P(1)–C(1)	111·7 (2)	P(1)–C(7)–C(12)	118·1 (5)
Au–P(1)–C(7)	113·3 (2)	P(2)–C(31)–C(32)	111·0 (4)
Au–P(1)–C(13)	113·3 (2)	P(2)–C(31)–C(36)	111·4 (4)
C(1)–P(1)–C(7)	105·3 (3)	P(1)–C(13)–C(14)	108·9 (4)
C(1)–P(1)–C(13)	108·2 (3)	P(1)–C(13)–C(18)	115·7 (4)
C(7)–P(1)–C(13)	104·6 (3)	P(2)–C(19)–C(20)	115·9 (4)
Au–P(2)–C(19)	116·7 (2)	P(2)–C(19)–C(24)	111·5 (5)
Au–P(2)–C(25)	111·8 (2)	P(2)–C(25)–C(26)	118·2 (4)
Au–P(2)–C(31)	111·7 (2)	P(2)–C(25)–C(30)	122·3 (5)
C(19)–P(2)–C(25)	104·0 (3)	C–C–C (Cy, ave.)	111·7 (7)
C(19)–P(2)–C(31)	106·6 (3)	C–C–C (Ph, ave.)	119·6 (7)
C(25)–P(2)–C(31)	105·2 (3)		

Cy_2PhP, 161·7° (calc.), distorted trigonal planar; Ph_3P, 145°, regular trigonal planar: cone angles from Tolman (1977)] which suggests that steric effects determine the coordination number and geometry of these complexes.
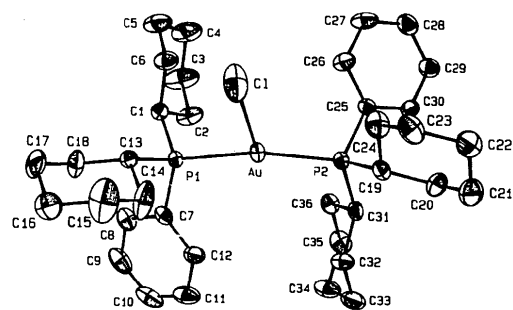
Fig. 1. Labeling of atoms in $[(Cy_2PhP)_2AuCl]$ (50% probability ellipsoids).
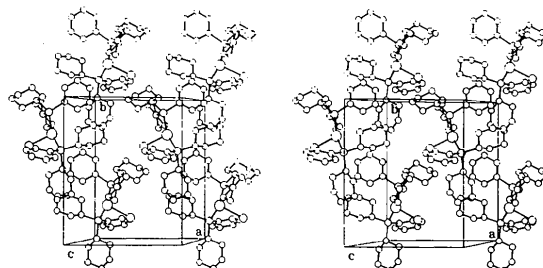
Fig. 2. Packing diagram of $[(Cy_2PhP)_2AuCl]$ in the unit cell.

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