C1—Au—P	178.56 (11)	C11—P—Au	113.92 (12)
C11—P—C21	106.6 (2)	C21—P—Au	113.38 (13)
C11—P—C31	104.9 (2)	C31—P—Au	110.45 (12)
C21—P—C31	107.0 (2)		

Program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1991). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1330). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Ahrland, S., Dreisch, K., Norén, B. & Oskarsson, Å. (1987). *Acta Chem. Scand. Ser. A*, **41**, 173–177.

Allen, F. H., Davies, J. E., Galloy, J. J., Johnson, O., Kennard, O., Macrae, C. F., Mitchell, E. M., Mitchell, G. F., Smith, J. M. & Watson, D. G. (1991). *J. Chem. Inf. Comput. Sci.* **31**, 187–204.

Barron, P. F., Engelhardt, L. M., Healy, P. C., Oddy, J. & White, A. H. (1987). *Aust. J. Chem.* **40**, 1545–1555.

Gavens, P. D., Guy, J. J., Mays, M. J. & Sheldrick, G. M. (1977). *Acta Cryst.* B**33**, 137–139.

Jones, P. G. & Lautner, J. (1988). *Acta Cryst.* C**44**, 2091–2093.

Murray, H. H., Fackler, J. P. Jr, Porter, L. C., Briggs, D. A., Guerra, M. A. & Lagow, R. J. (1987). *Inorg. Chem.* **26**, 357–363.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Siefert, R. (1994). Diploma thesis, Universität-GH Paderborn, Germany.

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$[Au(PPh_3)_2]^+[BF_4]^-$

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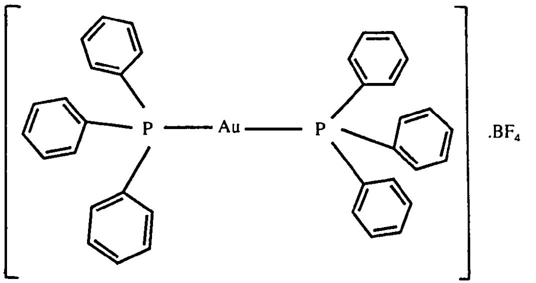
Abstract

The synthesis and structural characterization of the title compound, bis(triphenylphosphine)gold(I) tetrafluoroborate, $[Au(PPh_3)_2]^+[BF_4]^-$, are reported. The BF_4^- anion does not interact with the Au centre. The coordination geometry about Au is close to linear, with Au—P distances of 2.321 (3) and 2.322 (3) Å, and a P1—Au—P2 angle of 167.3 (1)°. The range of P—C distances is 1.787 (10)–1.823 (9) Å.

Comment

A number of mononuclear (King, Khan, Staples & Fackler, 1992, and references therein) and binuclear (Wang, Garzon, King, Wang & Fackler, 1989; King, Wang, Khan & Fackler, 1989) gold(I) compounds are luminescent. Structural information is essential for understanding this luminescent property. In this paper we report the crystal structure of $[Au(PPh_3)_2]^+[BF_4]^-$, (I).



(I)

The coordination number of the central Au atom is two, with two P atoms linearly bound to it. All four F atoms in the BF_4^- anion are disordered. Two other $[Au(PPh_3)_2]^+X^-$-type structures have been reported recently (X = NO_3, PF_6; Staples, King, Khan, Winpenny & Fackler, 1993). Fig. 1 shows a drawing of the molecule with the atom-labelling scheme.

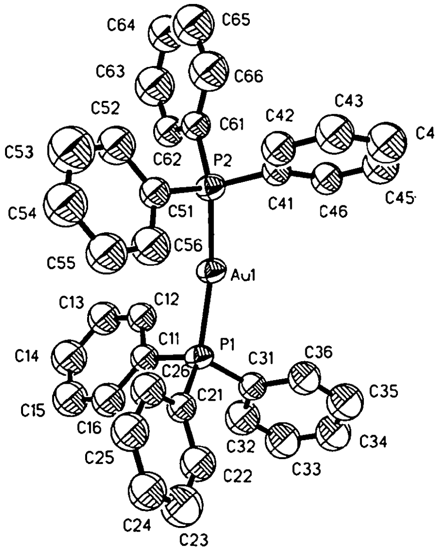


Fig. 1. Drawing (*SHELXTL-Plus*; Sheldrick, 1991) of the $[Au(PPh_3)_2]^+$ cation showing 50% probability ellipsoids for non-H atoms.

Experimental

The title compound was synthesized by reacting $[Au(PPh_3)_2]Cl$ with $AgBF_4$ in CH_2Cl_2 (DCM) and leaving overnight. After filtering off the precipitate, $[Au(PPh_3)_2]BF_4$ powders were formed by adding a large amount of diethyl ether (Et_2O) to the reaction solution. Colourless crystals of $[Au(PPh_3)_2]BF_4$ were grown from DCM/Et_2O mixed solvents.

Crystal data

$[Au(C_{18}H_{15}P)_2]BF_4$
$M_r = 808.3$
Monoclinic
$C2/c$
$a = 21.594\,(3)$ Å
$b = 12.399\,(2)$ Å
$c = 24.783\,(3)$ Å
$\beta = 92.10\,(2)°$
$V = 6631.0\,(15)$ Å^3
$Z = 8$
$D_x = 1.619$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10–15°$
$\mu = 4.580$ mm^{-1}
$T = 298$ K
Needle
$0.6 \times 0.2 \times 0.05$ mm
Colourless

Data collection

Siemens *P*4 diffractometer
$\theta/2\theta$ scans
Absorption correction: ψ scan (Siemens, 1989) $T_{\min} = 0.493$, $T_{\max} = 1.000$
4720 measured reflections
4337 independent reflections
2302 observed reflections [$I > 3\sigma(I)$]
$R_{\rm int} = 0.0233$

$\theta_{\max} = 22.5°$
$h = 0 \rightarrow 23$
$k = 0 \rightarrow 13$
$l = -26 \rightarrow 26$
3 standard reflections monitored every 300 reflections intensity decay: <2%

Refinement

Refinement on F
$R = 0.0395$
$wR = 0.0525$
$S = 1.03$
2302 reflections
124 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o) + 0.0015F_o^2]$
$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.87$ e Å^{-3}
$\Delta\rho_{\min} = -0.56$ e Å^{-3}
Extinction correction: $F^* = F[1 + (0.002\chi \times F^2/\sin 2\theta)]^{-1/4}$
Extinction coefficient: $8\,(6) \times 10^{-6}$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)*

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm iso}/U_{\rm eq}$
Au1	0.2456 (1)	0.0041 (1)	0.3867 (1)	0.047 (1)
P1	0.3355 (2)	0.1057 (3)	0.3964 (1)	0.045 (1)
P2	0.1589 (2)	−0.1036 (3)	0.3973 (1)	0.045 (1)
C12†	0.4063 (4)	−0.0457 (7)	0.3469 (3)	0.059 (4)
C13	0.4594	−0.1068	0.3389	0.077 (5)
C14	0.5108	−0.0962	0.3742	0.091 (5)
C15	0.5091	−0.0245	0.4176	0.086 (5)
C16	0.4559	0.0365	0.4255	0.073 (5)
C11	0.4045	0.0259	0.3902	0.052 (4)
C22	0.3668 (4)	0.2580 (7)	0.4768 (3)	0.073 (4)
C23	0.3718	0.2944	0.5301	0.100 (6)
C24	0.3498	0.2308	0.5717	0.078 (5)
C25	0.3228	0.1308	0.5600	0.078 (5)
C26	0.3179	0.0945	0.5068	0.069 (4)
C21	0.3399	0.1580	0.4652	0.052 (3)
C32	0.4044 (3)	0.2519 (7)	0.3380 (4)	0.081 (5)
C33	0.4109	0.3450	0.3071	0.091 (5)
C34	0.3589	0.4058	0.2917	0.088 (5)
C35	0.3003	0.3737	0.3074	0.089 (5)
C36	0.2937	0.2806	0.3383	0.069 (4)
C31	0.3458	0.2198	0.3536	0.049 (3)
C42	0.0389 (4)	−0.0490 (6)	0.4272 (3)	0.060 (4)
C43	−0.0172	0.0059	0.4200	0.075 (4)
C4	−0.0263	0.0763	0.3765	0.082 (5)
C45	0.0208	0.0917	0.3402	0.075 (4)
C46	0.0768	0.0368	0.3473	0.056 (4)
C41	0.0859	−0.0336	0.3908	0.047 (3)
C52	0.1465 (5)	−0.2602 (7)	0.4786 (3)	0.077 (5)
C53	0.1476	−0.2939	0.5323	0.111 (6)
C54	0.1644	−0.2217	0.5735	0.092 (5)
C55	0.1801	−0.1158	0.5609	0.082 (5)
C56	0.1791	−0.0820	0.5072	0.078 (5)
C51	0.1623	−0.1543	0.4660	0.050 (3)
C62	0.2012 (3)	−0.2617	0.3295 (4)	0.059 (4)
C63	0.1953	−0.3562	0.2992	0.099 (6)
C64	0.1378	−0.4069	0.2931	0.086 (5)
C65	0.0862	−0.3632	0.3173	0.101 (6)
C66	0.0921	−0.2688	0.3477	0.091 (5)
C61	0.1496	−0.2180	0.3538	0.049 (3)
B1‡	0.3556 (3)	−0.2649 (5)	0.2452 (3)	0.092 (7)
F1	0.3176	−0.3462	0.2266	0.094 (4)
F2	0.3287	−0.2134	0.2873	0.104 (7)
F3	0.3647	−0.1927	0.2044	0.093 (6)
F4	0.4114	−0.3073	0.2626	0.099 (6)
F1′	0.3244	−0.3308	0.2091	0.094 (4)
F2′	0.3198	−0.1766	0.2557	0.121 (7)
F3′	0.4100	−0.2319	0.2238	0.166 (10)
F4′	0.3680	−0.3202	0.2922	0.149 (9)

† Phenyl rings were refined as rigid groups with isotropic displacement parameters for the C atoms. ‡ Disordered BF_4 anion refined isotropically with partially occupied F sites (see below).

Table 2. *Selected geometric parameters (Å, °)*

Au1—P1	2.321 (3)	Au1—P2	2.322 (3)
P1—C11	1.800 (9)	P1—C21	1.823 (9)
P1—C31	1.787 (10)	P2—C41	1.801 (9)
P2—C51	1.815 (9)	P2—C61	1.789 (9)
P1—Au1—P2	167.3 (1)	Au1—P1—C11	112.7 (3)
Au1—P1—C21	107.8 (3)	C11—P1—C21	105.2 (4)
Au1—P1—C31	119.3 (3)	C11—P1—C31	105.2 (4)
C21—P1—C31	105.6 (4)	Au1—P2—C41	114.8 (3)
Au1—P2—C51	107.5 (3)	C41—P2—C51	104.8 (4)
Au1—P2—C61	117.4 (3)	C41—P2—C61	104.5 (4)
C51—P2—C61	106.9 (4)	P1—C11—C12	117.5 (3)

The structure was solved by the Patterson method using *SHELXTL-Plus* (Sheldrick, 1991). All C atoms on the phenyl rings were refined as rigid groups. The BF_4 anion was disordered, and was represented by two sets of four F atoms, sharing a common B centre. H atoms were placed in idealized positions. These H atoms were included in the structure-factor calculations but were not included in the least-squares calculations.

These studies were supported by the National Science Council (NSC81-0208-M031-001) of the Republic of China.

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: HU1080). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

King, C., Khan, M. N. I., Staples, R. J. & Fackler, J. P. Jr (1992). *Inorg. Chem.* **31**, 3236–3238.
King, C., Wang, J.-C., Khan, M. N. I. & Fackler, J. P. Jr (1989). *Inorg. Chem.* **28**, 2145–2148.

Sheldrick, G. M. (1991). *SHELXTL-Plus*. Release 4.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1989). Diffractometer software. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Staples, R. J., King, C., Khan, M. N. I., Winpenny, E. P. & Fackler, J. P. Jr (1993). *Acta Cryst.* C**49**, 472–475.
Wang, S., Garzon, G., King, C., Wang, J.-C. & Fackler, J. P. Jr (1989). *Inorg. Chem.* **28**, 4263–4269.

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Tricarbonyl(η^6-1-tetralol)chromium

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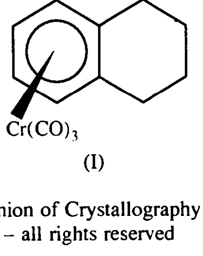
Abstract

In the structure of tricarbonyl(η^6-1,2,3,4-tetrahydro-1-naphthalenol)chromium, [$Cr(CO)_3(C_{10}H_{12}O)$], the group of three carbonyl ligands is *syn* with respect to the hydroxy group. The asymmetric unit contains two molecules of the same enantiomer with no significant differences in terms of intramolecular bond lengths and bond angles. The $Cr(CO)_3$ tripod is complexed to the benzene ring in an eclipsed conformation. An extensive hydrogen-bonding network supports the crystal structure.

Comment

Tricarbonylchromium-complexed organic molecules receive much attention as intermediates in asymmetric syntheses (Solladie-Cavallo, 1989). In order to determine the absolute stereochemistry of the final metal-free targets, it is essential to know the spatial structure of the complexes. Tricarbonyl(η^6-1-tetralol)chromium, (I), has been prepared previously (Jaouen & Meyer, 1975; Davies & Goodfellow, 1988; Schmalz, Millies, Bats & Dürner, 1992) but, to date, the *syn* configuration of the tricarbonyl tripod with respect to the hydroxy group has been established only by indirect methods. This structure determination has confirmed the previous results.



(I)

The asymmetric unit contains two molecules of the same enantiomer with no significant differences in the intramolecular bond lengths and bond angles. The $Cr(CO)_3$ group is complexed to the benzene ring (Fig. 1) in an eclipsed conformation with the carbonyl groups located near the C10, C8 and C12 (C10′, C8′ and C12′) atoms (Fig. 2); this means that the C8—C7 (C8′—C7′) bond, connecting the more electron-donating C7 (C7′) substituent, is eclipsed with respect to the C3—O3 (C3′—O3′) carbonyl group, as would be expected considering the electronic properties of this kind of compound (Muetterties, Bleeke, Wucherer & Albright, 1982). The Cr—C(arene) distances range between 2.201 (3) and 2.256 (3) Å with the highest values for the substituted atoms C8 and C9 (C8′ and C9′). The largest deviation from the least-square plane of the benzene ring is 0.016 (4) Å for atom C11′ [0.012 (3) Å for C11], while the substituent atoms C4 and C7 lie at 0.028 (3) and 0.019 (4) Å, respectively [0.018 (3) and 0.014 (3) Å for C4′ and C7′] from the plane on the opposite side with respect to the $Cr(CO)_3$ group.

There is an extensive hydrogen-bonding network within the crystal (Fig. 3); the two molecules in the asymmetric unit are linked by a hydrogen bond between H4O and O4′ [H4O···O4′ 2.08 (4), O4···O4′ 2.848 (3) Å, O4—H4O···O4′ 166 (3)°]. Another hydrogen bond links the asymmetric unit to the nearest molecules [H4O′···O4[i] 2.07 (4), O4′···O4[i] 2.878 (3) Å, O4′—H4O′···O4[i] 170 (3)°; symmetry code: (i) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$].

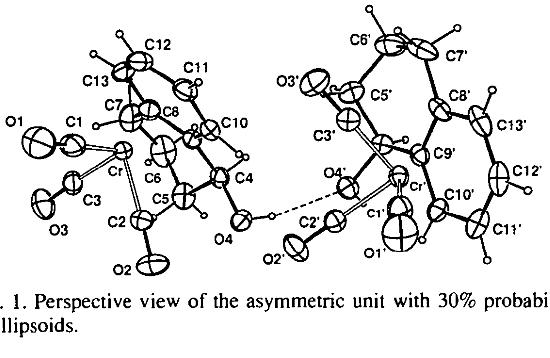


Fig. 1. Perspective view of the asymmetric unit with 30% probability ellipsoids.

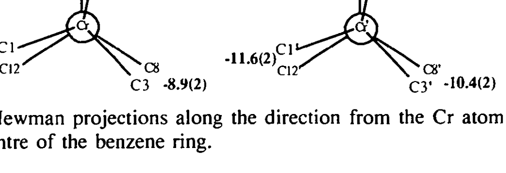


Fig. 2. Newman projections along the direction from the Cr atom to the centre of the benzene ring.