

atoms deviate more from the plane through [Pdphen₂]²⁺ than do N(1), C(1), and C(2) (Table 1).

Cl—O distances range from 1.356 to 1.417 Å. The O atoms are very anisotropic. Correction of bond lengths assuming riding motion (Busing & Levy, 1964) gives minimum values of 1.410, 1.413, 1.439 and 1.425 Å, giving a mean value of 1.422 (3) Å, *cf.* 1.433 (3) Å in KClO₄ (Johansson & Lindqvist, 1977).

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Tris(triphenylphosphine)gold(I) Tetraphenylborate

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Abstract. C₅₄H₄₅AuP₃⁺·C₂₄H₂₀B₄⁻, [Au(C₁₈H₁₅P)₃][B(C₆H₅)₄], *M_r* = 1241.13, monoclinic, *P*2₁/*c*, *a* = 16.747 (6), *b* = 20.645 (8), *c* = 18.398 (7) Å, β = 95.06 (2)°, *U* = 6336 Å³, *Z* = 4, *D_x* = 1.301 Mg m⁻³, μ(Mo *Kα*) = 2.4 mm⁻¹. Final *R* = 0.054 for 8753 reflexions. The Au atom shows trigonal planar coordination with Au—P 2.365 (3), 2.384 (3), 2.403 (3) Å, and P—Au—P 115.2 (2), 119.3 (2), 125.4 (2)°.

Introduction. During attempts to recrystallize L₄Au⁺·BPh₄⁻ (*L* = PPh₃ throughout this paper), large colourless crystals were obtained from acetonitrile. The approximate cell volume, determined from preliminary photographs, indicated that one ligand had been lost. In view of the paucity of information on three-coordinate Au^I complexes, a crystal structure determination was undertaken.

Data were collected on a Stoe four-circle diffractometer with a profile-fitting method (Clegg, 1981).

11 522 intensities were measured in the range 7 < 2θ < 55° (monochromated Mo *Kα* radiation). After *L_p* and empirical absorption corrections (crystal size 0.75 × 0.35 × 0.2 mm), averaging equivalent reflexions gave 8753 unique data with *F* > 4σ(*F*).

The structure was solved by the heavy-atom method and refined to *R_w* = ∑*w*^{1/2}Δ/∑*w*^{1/2}|*F_o*| = 0.054 = *R*. The weighting scheme was *w*⁻¹ = σ²(*F*) + 0.0005*F*². The Au and P atoms were anisotropic; the phenyl rings were treated as rigid groups with C—C 1.395, C—H 0.96 Å and all angles 120°, *U*(H) = 1.2*U*(C). Final atomic coordinates are given in Table 1, bond lengths and angles in Table 2.* A final difference map showed no peaks > 1 e Å⁻³.

* Lists of structure factors, H atom coordinates and anisotropic temperature factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35589 (56 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i>
Au	2173 (1)	4307 (1)	7213 (1)	40 (1)*
P(1)	2415 (1)	5376 (1)	6823 (1)	40 (1)*
P(2)	2144 (1)	3438 (1)	6343 (1)	42 (1)*
P(3)	2048 (1)	3986 (1)	8442 (1)	41 (1)*
C(112)	2654 (3)	5901 (2)	8200 (3)	70 (2)
C(113)	2676 (3)	6396 (2)	8718 (3)	85 (3)
C(114)	2408 (3)	7015 (2)	8516 (3)	90 (3)
C(115)	2118 (3)	7140 (2)	7795 (3)	74 (2)
C(116)	2096 (3)	6646 (2)	7277 (3)	59 (2)
C(111)	2364 (3)	6026 (2)	7479 (3)	46 (2)
C(122)	3753 (3)	4913 (2)	6218 (2)	54 (2)
C(123)	4512 (3)	4956 (2)	5964 (2)	67 (2)
C(124)	4910 (3)	5549 (2)	5973 (2)	70 (2)
C(125)	4550 (3)	6101 (2)	6237 (2)	63 (2)
C(126)	3791 (3)	6058 (2)	6491 (2)	55 (2)
C(121)	3393 (3)	5464 (2)	6482 (2)	42 (1)
C(132)	1913 (2)	5861 (2)	5418 (2)	58 (2)
C(133)	1325 (2)	6026 (2)	4865 (2)	77 (2)
C(134)	517 (2)	5934 (2)	4966 (2)	76 (2)
C(135)	297 (2)	5675 (2)	5620 (2)	83 (3)
C(136)	885 (2)	5509 (2)	6173 (2)	65 (2)
C(131)	1693 (2)	5602 (2)	6072 (2)	42 (1)
C(212)	1999 (2)	4136 (2)	5057 (2)	57 (2)
C(213)	2197 (2)	4315 (2)	4364 (2)	67 (2)
C(214)	2819 (2)	4001 (2)	4051 (2)	66 (2)
C(215)	3244 (2)	3507 (2)	4431 (2)	71 (2)
C(216)	3047 (2)	3328 (2)	5124 (2)	62 (2)
C(211)	2424 (2)	3643 (2)	5437 (2)	46 (2)
C(222)	620 (3)	3100 (2)	6661 (2)	58 (2)
C(223)	-103 (3)	2761 (2)	6562 (2)	75 (2)
C(224)	-251 (3)	2350 (2)	5964 (2)	81 (2)
C(225)	322 (3)	2277 (2)	5465 (2)	80 (2)
C(226)	1045 (3)	2615 (2)	5563 (2)	70 (2)
C(221)	1193 (3)	3027 (2)	6161 (2)	49 (2)
C(232)	3581 (3)	3046 (2)	7030 (3)	74 (2)
C(233)	4160 (3)	2606 (2)	7309 (3)	101 (3)
C(234)	4021 (3)	1942 (2)	7236 (3)	93 (3)
C(235)	3302 (3)	1719 (2)	6883 (3)	100 (3)
C(236)	2722 (3)	2159 (2)	6604 (3)	73 (2)
C(231)	2861 (3)	2823 (2)	6678 (3)	50 (2)
C(312)	1810 (3)	4678 (2)	9738 (2)	69 (2)
C(313)	1426 (3)	5145 (2)	10132 (2)	93 (3)
C(314)	829 (3)	5533 (2)	9780 (2)	89 (3)
C(315)	615 (3)	5455 (2)	9035 (2)	89 (3)
C(316)	999 (3)	4988 (2)	8642 (2)	72 (2)
C(311)	1596 (3)	4600 (2)	8993 (2)	46 (2)
C(322)	1770 (2)	2658 (2)	8382 (3)	63 (2)
C(323)	1282 (2)	2110 (2)	8323 (3)	87 (3)
C(324)	462 (2)	2166 (2)	8390 (3)	84 (3)
C(325)	130 (2)	2772 (2)	8516 (3)	76 (2)
C(326)	618 (2)	3320 (2)	8574 (3)	63 (2)
C(321)	1438 (2)	3263 (2)	8507 (3)	49 (2)
C(332)	3696 (2)	4024 (2)	8606 (2)	51 (2)
C(333)	4459 (2)	3878 (2)	8931 (2)	60 (2)
C(334)	4545 (2)	3491 (2)	9554 (2)	61 (2)
C(335)	3867 (2)	3250 (2)	9853 (2)	64 (2)
C(336)	3104 (2)	3396 (2)	9528 (2)	57 (2)
C(331)	3019 (2)	3783 (2)	8904 (2)	45 (2)
C(412)	3574 (2)	9748 (2)	6043 (2)	54 (2)
C(413)	4109 (2)	10164 (2)	5737 (2)	61 (2)
C(414)	4743 (2)	10438 (2)	6176 (2)	65 (2)
C(415)	4841 (2)	10296 (2)	6919 (2)	64 (2)
C(416)	4306 (2)	9880 (2)	7225 (2)	54 (2)
C(411)	3672 (2)	9606 (2)	6786 (2)	45 (1)
C(422)	2017 (2)	8362 (2)	6250 (3)	59 (2)

Table 1 (cont.)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i>
C(423)	1891 (2)	7877 (2)	5725 (3)	75 (2)
C(424)	2542 (2)	7549 (2)	5477 (3)	74 (2)
C(425)	3320 (2)	7706 (2)	5753 (3)	75 (2)
C(426)	3447 (2)	8191 (2)	6279 (3)	66 (2)
C(421)	2795 (2)	8519 (2)	6527 (3)	52 (2)
C(432)	2073 (3)	10175 (2)	7037 (3)	65 (2)
C(433)	1394 (3)	10528 (2)	7181 (3)	74 (2)
C(434)	808 (3)	10244 (2)	7572 (3)	76 (2)
C(435)	902 (3)	9608 (2)	7819 (3)	80 (2)
C(436)	1580 (3)	9254 (2)	7675 (3)	67 (2)
C(431)	2166 (3)	9538 (2)	7284 (3)	52 (2)
C(442)	3345 (3)	9216 (2)	8569 (3)	67 (2)
C(443)	3702 (3)	9010 (2)	9243 (3)	80 (2)
C(444)	4089 (3)	8411 (2)	9303 (3)	90 (3)
C(445)	4119 (3)	8019 (2)	8689 (3)	106 (3)
C(446)	3762 (3)	8226 (2)	8014 (3)	86 (3)
C(441)	3375 (3)	8824 (2)	7955 (3)	52 (2)
B	2994 (5)	9112 (4)	7143 (4)	46 (2)

* U_{eq} is $\frac{1}{3}$ of the trace of the orthogonalized **U** matrix.

Table 2. Bond lengths (\AA) and angles ($^\circ$)

Au—P(1)	2.365 (3)	Au—P(2)	2.403 (3)
Au—P(3)	2.384 (3)	C(111)—P(1)	1.813 (6)
C(121)—P(1)	1.814 (6)	C(131)—P(1)	1.815 (5)
C(211)—P(2)	1.821 (6)	C(221)—P(2)	1.809 (6)
C(231)—P(2)	1.817 (6)	C(311)—P(3)	1.829 (6)
C(321)—P(3)	1.819 (6)	C(331)—P(3)	1.815 (5)
B—C(411)	1.700 (10)	B—C(421)	1.681 (10)
B—C(431)	1.682 (10)	B—C(441)	1.681 (10)
P(1)—Au—P(2)	119.3 (2)	P(1)—Au—P(3)	125.4 (2)
P(2)—Au—P(3)	115.2 (2)	Au—P(1)—C(111)	118.0 (3)
Au—P(1)—C(121)	112.5 (2)	C(111)—P(1)—C(121)	104.6 (3)
Au—P(1)—C(131)	110.5 (3)	C(111)—P(1)—C(131)	104.4 (3)
C(121)—P(1)—C(131)	105.8 (3)	Au—P(2)—C(211)	116.4 (3)
Au—P(2)—C(221)	116.0 (3)	C(211)—P(2)—C(221)	103.5 (3)
Au—P(2)—C(231)	108.8 (3)	C(211)—P(2)—C(231)	104.9 (3)
C(221)—P(2)—C(231)	106.3 (3)	Au—P(3)—C(311)	114.1 (3)
Au—P(3)—C(321)	112.8 (3)	C(311)—P(3)—C(321)	105.7 (3)
Au—P(3)—C(331)	111.0 (2)	C(311)—P(3)—C(331)	107.3 (3)
C(321)—P(3)—C(331)	105.4 (3)	P(1)—C(111)—C(112)	117.6 (2)
P(1)—C(111)—C(116)	122.3 (2)	P(1)—C(121)—C(122)	118.0 (2)
P(1)—C(121)—C(126)	122.0 (2)	P(1)—C(131)—C(132)	123.1 (2)
P(1)—C(131)—C(136)	116.9 (2)	P(2)—C(211)—C(212)	117.9 (2)
P(2)—C(211)—C(216)	122.1 (2)	P(2)—C(221)—C(222)	118.3 (2)
P(2)—C(221)—C(226)	121.6 (2)	P(2)—C(231)—C(232)	116.4 (3)
P(2)—C(231)—C(236)	123.6 (3)	P(3)—C(311)—C(312)	122.9 (2)
P(2)—C(311)—C(316)	117.1 (2)	P(3)—C(321)—C(322)	119.3 (2)
P(3)—C(321)—C(326)	120.0 (2)	P(3)—C(331)—C(332)	117.3 (2)
P(3)—C(331)—C(336)	122.7 (2)	C(412)—C(411)—B	118.6 (4)
C(416)—C(411)—B	121.4 (4)	C(422)—C(421)—B	122.6 (4)
C(426)—C(421)—B	117.4 (4)	C(432)—C(431)—B	120.8 (4)
C(436)—C(431)—B	119.2 (4)	C(442)—C(441)—B	118.5 (4)
C(446)—C(441)—B	121.4 (4)	C(411)—B—C(421)	106.1 (6)
C(411)—B—C(431)	109.5 (6)	C(421)—B—C(431)	111.6 (6)
C(411)—B—C(441)	109.9 (6)	C(421)—B—C(441)	112.2 (6)
C(431)—B—C(441)	107.5 (6)		

Discussion. The structure determination confirms the compound as $L_3Au^+ \cdot BPh_4^-$. The cation is shown in Fig. 1. The coordination of the Au atom is trigonal planar (see Table 2); it lies 0.06 \AA out of the P_3 plane.

Examples of regular three-coordination for Au^I are few; the usual tendency is for one ligand to be weakly bonded, leading to distortion of ideal geometry. Thus,

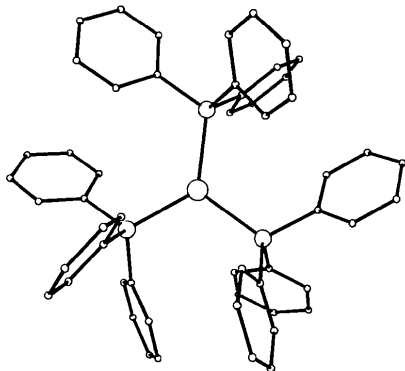


Fig. 1. The $[\text{Au}(\text{Ph}_3\text{P})_3]^+$ cation.

in $[\text{Au}(\text{SnCl}_3)(\text{Me}_2\text{PhP})_2]$ (Clegg, 1978) a long Au—Sn bond of 2.881 (1) Å is reflected in a wide P—Au—P angle of 153.8 (2)°. The compounds $L_2\text{Au}X$ [$X = \text{Cl}$ (Baenziger, Dittmore & Doyle, 1974), and $X = \text{I}$ (Beindorf & Strähle, 1980)] also exhibit P—Au—P angles wider than ideal [132.1 (1), 131.2 (3)° respectively], and the chloride shows a long Au—Cl bond of 2.500 (4) Å. The Au—I bond of the iodide is 2.776 (2) Å; no Au—I bonds are available for comparison. More regular geometry is only attained with three identical ligands, e.g. in the ternary compounds $\text{Au}_7\text{P}_{10}\text{I}$, possessing trigonal AuP_3 moieties with Au—P 2.339 (7) Å, P—Au—P 118.5 (2)°, site symmetry $3m$ (Jeitschko & Möller, 1979), and $\text{Ti}_6\text{Au}_2\text{I}_{10}$, possessing AuI_3 units with Au—I 2.74 (1), 2.81 (1) Å, all angles 120°, site symmetries 32 and $\bar{6}$ respectively (Stoeger & Rabenau, 1979). The only non-polymeric structure with three identical ligands is $L_3\text{Au}^+\cdot\text{B}_9\text{H}_9\text{S}^-$ (Guggen-

berger, 1974). Despite the fact that this cation and that of the present compound are formally identical, they display significant structural differences. The thiadecaborate derivative displays less regular geometry, with Au—P 2.345, 2.384, 2.389 Å, P—Au—P 112.3, 121.5, 124.1°; the Au atom lies 0.2 Å out of the P_3 plane. (The first of these bond lengths was reported as 2.373 Å, but this is not consistent with the atomic coordinates and cell constants.) Differing phenyl-ring orientations in the two cations suggest that packing forces may be responsible for their structural differences. Neither compound displays unusually short non-bonded distances.

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Iron(II) Formate Dihydrate

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Abstract. $\text{Fe}(\text{HCO}_2)_2 \cdot 2\text{H}_2\text{O}$, $2\text{CHO}_2^- \cdot \text{Fe}^{2+} \cdot 2\text{H}_2\text{O}$, $M_r = 181.91$, monoclinic, $P2_1/c$, $a = 8.740$ (3), $b = 7.192$ (3), $c = 9.428$ (4) Å, $\beta = 97.47$ (2)°, $Z = 4$, $D_c = 2.056$ Mg m⁻³, $\mu_{\text{MoK}\alpha} = 2.483$ mm⁻¹, $R = 0.032$, $R_w = 0.028$ for 1319 independent reflexions. The compound is isostructural with isomorphous formate dihydrates of other bivalent metals; coordination distances range from 2.084 (2) to 2.180 (2) Å.

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Introduction. The isomorphous formate dihydrates of Mg (de With, Harkema & van Hummel, 1976), Zn (Burger & Fuess, 1977), Cd (Post & Trotter, 1974), Co^{II} (Antsyshkina, Guseinova & Porai-Koshits, 1967), Ni^{II} (Krogmann & Mattes, 1963), Cu^{II} (Bukowska-Strzyżewska, 1965; Kay, Almodovar & Kaplan, 1968), Mn^{II} (Osaki, Nakai & Watanabé, 1964; Kay, Almodovar & Kaplan, 1968) and Fe^{II} (Hoy, de S.

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