of the two Zn atoms in $Zn(Gly)_2.H_2O$ as having an 'approximately square-pyramidal' coordination geometry (see above) is an over-simplification. In terms of the criteria proposed by Auf der Heyde & Nassimbeni for five-coordinate Zn complexes, the angles at both Zn(1) and Zn(2) lie between the values for trigonal-bipyramidal (tbp) and square-pyramidal (sp) geometries.* Appropriate calculations show that both Zn atoms lie on the Berry coordinate of Fig. 5 in the cited reference, the tbp:sp ratios being 47:53 for Zn(1) and 33:67 for Zn(2), respectively.† The shallowness of the free-energy minimum for five-coordinate Zn is illustrated by the fact that two Zn sites with significantly different geometries lying on the Berry coordinate occur in the same unit cell.

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* The ligand atoms corresponding to positions 1–5 in the scheme of Auf der Heyde & Nassimbeni (1984) are: Zn(1) – O(1), N(1), O(8), N(2), O(3); Zn(2) – O(5), N(3), O(4), N(4), O(7). In the description of a tbp complex, positions 1 and 5 are axial, and positions 2, 3 and 4 are equatorial. In the description of an sp complex, position 3 is the apex of the pyramid and positions 1, 2, 4 and 5 are adjacent corners of the base.

† While our description of the glycinate ligand configurations as 'trans-N(amino)–trans-O(carboxyl)' would be inappropriate in a tbp complex, it remains intact since the coordination geometries of Zn(1) and Zn(2) are more sp than tbp.

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trans-Chlorohydridobis[tris(p-tolyl)phosphine]platinum(II)

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Abstract. [Pt(Cl)(H)($C_{21}H_{21}P$)$_2$], $M_r = 840.30$, triclinic, $P\bar{1}$, $a = 11.336$ (4), $b = 16.682$ (3), $c = 11.049$ (2) Å, $\alpha = 103.03$ (2), $\beta = 113.32$ (2), $\gamma = 85.87$ (2)°, $V = 1868.9$ (1.8) Å^3, $Z = 2$, $D_x = 1.49$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 39.8$ cm^{-1}, $F(000) = 840$, $T = 294$ (1) K, $R = 0.041$ for 5149 unique reflections with $F^2 > 3\sigma(F^2)$ of 7313 total unique data. Principal bond lengths (Å) and angles (°) are: Pt—P 2.278 (2), 2.282 (2); Pt—Cl 2.384 (3); P—Pt—P 167.18 (9); Cl—Pt—P 94.52 (8), 97.98 (8).

Introduction. Hydride complexes of platinum(II) exhibit a rich and varied chemistry, including applications in homogeneous catalysis (Hartley, 1973, and references therein). Among the well-known series of trans-[PtH(X)(PR_3)$_2$] complexes, the complex trans-[PtH(Cl)(PPh$_3$)$_2$] (1), containing stabilizing triarylphosphine ligands, has perhaps been the most studied example in synthetic and catalytic work. Attempts to completely characterize this complex by X-ray crystallography have been largely unsuccessful, although a preliminary report (Bender, Braunstein, Jud & Dusausory, 1984) of a determination using a poor-quality crystal was made in 1984. Here we describe the structure of a close relative, trans-[PtH(Cl){P(p-tolyl)$_3$}$_2$] (2), where the presence of the

methyl ring substituents not only allows good-quality crystals to be obtained, but also provides a convenient probe for monitoring solution chemistry by ^{1}H and ^{13}C{^{1}H} NMR methods. Crystals of the title compound were obtained from an attempted synthesis of [Pt(C≡CH)$_2${P(p-tolyl)$_3$}$_2$] where acetylene was bubbled through a basic, ethanolic solution (NaH/ethanol) of cis-[PtCl$_2${P(p-tolyl)$_3$}$_2$] (3). Instead of isolating the acetylide complex, the title compound was formed in good yield. We found that bubbling the basic, ethanolic solution of (3) with acetylene is not necessary to form the hydride which is probably produced via initial generation of an ethoxide complex, followed by β-hydride elimination. Indeed, directly monitoring the reaction of (3) with NaH/ethanol by ^{31}P{^{1}H}-NMR spectroscopy with no acetylene present allowed the conversion of (3) to (2) to be monitored. No intermediates were detected.

Experimental. Sodium hydride (Alfa, powder, 7·4 mg) was added to anhydrous ethanol (30 mL) under dry nitrogen and bubbled with scrubbed acetylene for 5 min. Complex (3) (271 mg) was added and the suspension bubbled with acetylene for a further 5 min. The suspension was then filtered to remove residual starting material (confirmed by ^{31}P{^{1}H} NMR) and the orange filtrate refrigerated. After 2 days, 160 mg of light-orange crystalline material was collected by filtration. The product was characterized as (2) (61·4% yield) spectroscopically: ^{31}P{^{1}H} NMR: $\delta = 25\cdot9$ vs H$_3$PO$_4$, $^1J(^{195}$Pt,^{31}P) = 3000 Hz [$cf.$ literature data for (1): $\delta = 111\cdot7$ vs P(OMe)$_3$, $i.e.$ $\delta = 29\cdot3$ vs H$_3$PO$_4$, $^1J(^{195}$Pt,^{31}P) = 3008 Hz]. ^{1}H NMR: δ(Pt—H) = $-15\cdot3$, $^1J(^{195}$Pt,^{1}H) = 1177, $^2J(^{31}$P,^{1}H) = 14 Hz [$cf.$ literature data for (1): $\delta = -16\cdot1$, $^1J(^{195}$Pt,^{1}H) = 1194, $^2J(^{31}$P,^{1}H) = 13 Hz]; δ(aromatic) = 7·94 (mult); 6·90 (d, $J =$ 7·6 Hz); δ(CH$_3$) = 1·95 (s). IR: ν(Pt—H) = 2238 cm^{-1} [$cf.$ literature data for (1): ν(Pt—H) = 2217 cm^{-1}]. Elemental analysis gave satisfactory values for C and H, but unexpectedly low values for Cl. Calc. (found) (%): C 60·03 (59·85), H 5·16 (5·21), Cl 4·22 (2·65). Repetition of this synthesis without the use of acetylene gave essentially identical results. Literature spectroscopic data for (1) are taken from Eaborn, Pidcock & Steele (1976) and Collamati, Furlani & Attioli (1970).

An essentially colorless hexagonal plate crystal was selected for X-ray analysis. Crystal 0·30 × 0·20 × 0·05 mm; Enraf–Nonius CAD-4 computer-controlled κ-axis diffractometer, graphite monochromator; cell dimensions from 25 reflections, 11° < θ < 13°; $a = 11\cdot336$ (4), $b = 16\cdot682$ (3), $c = 11\cdot049$ (2) Å, $\alpha = 103\cdot03$ (2), $\beta = 113\cdot32$ (2), $\gamma = 85\cdot87$ (2)°; standard reduced cell: $a = 11\cdot049$ (2), $b = 11\cdot336$ (4), $c = 16\cdot682$ (3) Å, $\alpha = 85\cdot87$ (2), $\beta =$

76·97 (2), $\gamma = 66\cdot68$ (2)°; transformation matrix: [0, -1, 0/0, 0, -1/100]; ω–2θ scan type; relative transmission coefficients, range 0·887–1·000; max. 2θ = 52°; h 0 to 14, k -20 to 20, l -12 to 12; three standard reflections, average decay 14·6%, anisotropic decay correction applied; 7326 data, 7313 unique, $R_{int} = 0\cdot032$; structure solved by Patterson and Fourier methods; refined by full-matrix least squares minimizing $\Sigma w(|F_o| - |F_c|)^2$, $w = 4F_o^2/\sigma^2(F_o)$ {$\sigma^2(F_o^2) = [s^2(c + R^2B) + (pF_o^2)^2]/\text{Lp}^2$}, using 5149 reflections with $F^2 > 3\sigma(F^2)$, 415 parameters; H atoms (including the hydride) in calculated positions (Pt—H = 1·70, C—H = 0·95 Å; CH$_3$ groups were assumed to be disordered between two possible conformations) refined as riding atoms with fixed isotropic thermal parameters [U(H) = 1·3 × U(bonded atom)], anisotropic thermal parameters for non-H atoms; final $R = 0\cdot041$, $wR = 0\cdot060$; maximum shift to e.s.d. = 0·08; max. and min. of ΔF synthesis 1·28

Table 1. *Positional and equivalent isotropic thermal parameters with e.s.d.'s in parentheses*

	x	y	z	$B(\text{Å}^2)$
Pt(1)	0·07248 (3)	0·23607 (2)	0·24133 (3)	2·974 (6)
Cl(1)	0·1443 (3)	0·3300 (2)	0·1500 (3)	7·34 (7)
P(1)	−0·1155 (2)	0·2033 (1)	0·0581 (2)	2·99 (4)
P(2)	0·2395 (2)	0·2543 (1)	0·4471 (2)	2·82 (4)
C(1)	0·1872 (7)	0·3131 (4)	0·5765 (7)	2·8 (2)
C(2)	0·2039 (8)	0·2880 (5)	0·6934 (7)	3·8 (2)
C(3)	0·1560 (8)	0·3347 (5)	0·7841 (7)	4·1 (2)
C(4)	0·0945 (8)	0·4058 (5)	0·7633 (8)	3·9 (2)
C(5)	0·0758 (8)	0·4312 (5)	0·6446 (8)	3·9 (2)
C(6)	0·1204 (8)	0·3847 (5)	0·5517 (7)	3·6 (2)
C(7)	0·044 (1)	0·4539 (8)	0·866 (1)	6·7 (3)
C(8)	0·3024 (7)	0·1597 (5)	0·5030 (7)	3·1 (2)
C(9)	0·4197 (9)	0·1594 (6)	0·6117 (8)	4·3 (2)
C(10)	0·4656 (8)	0·0873 (6)	0·6547 (8)	4·3 (2)
C(11)	0·3970 (8)	0·0134 (6)	0·5922 (8)	4·3 (2)
C(12)	0·2842 (9)	0·0143 (6)	0·487 (1)	5·0 (3)
C(13)	0·2351 (8)	0·0858 (5)	0·4397 (8)	4·3 (2)
C(14)	0·445 (1)	−0·0651 (6)	0·639 (1)	5·9 (3)
C(15)	0·3824 (7)	0·3094 (5)	0·4713 (7)	3·2 (2)
C(16)	0·4348 (8)	0·2881 (6)	0·3729 (8)	4·2 (2)
C(17)	0·5433 (8)	0·3280 (7)	0·3876 (9)	5·1 (2)
C(18)	0·6069 (8)	0·3884 (6)	0·499 (1)	5·0 (2)
C(19)	0·556 (1)	0·4086 (7)	0·596 (1)	6·4 (3)
C(20)	0·4454 (9)	0·3701 (6)	0·584 (1)	5·6 (3)
C(21)	0·722 (1)	0·4328 (8)	0·513 (1)	8·0 (4)
C(22)	−0·1818 (7)	0·1013 (5)	0·0362 (7)	3·3 (2)
C(23)	−0·1944 (9)	0·0369 (5)	−0·0711 (8)	4·2 (2)
C(24)	−0·2422 (9)	−0·0390 (5)	−0·0788 (8)	4·5 (2)
C(25)	−0·2845 (8)	−0·0520 (5)	0·0168 (8)	4·3 (2)
C(26)	−0·272 (1)	0·0124 (6)	0·1209 (9)	5·8 (2)
C(27)	−0·2186 (9)	0·0875 (6)	0·1360 (8)	5·3 (2)
C(28)	−0·341 (1)	−0·1337 (6)	0·005 (1)	6·0 (3)
C(29)	−0·1138 (7)	0·2022 (5)	−0·1065 (7)	3·3 (2)
C(30)	−0·0193 (8)	0·1603 (6)	−0·1383 (8)	4·4 (2)
C(31)	−0·0169 (9)	0·1547 (7)	−0·2656 (8)	5·2 (2)
C(32)	−0·1061 (9)	0·1907 (6)	−0·3588 (8)	5·6 (2)
C(33)	−0·201 (1)	0·2346 (6)	−0·3253 (8)	5·4 (2)
C(34)	−0·2049 (9)	0·2395 (6)	−0·2005 (8)	4·8 (2)
C(35)	−0·104 (1)	0·1862 (9)	−0·4952 (9)	8·0 (3)
C(36)	−0·2443 (7)	0·2709 (5)	0·0679 (7)	3·5 (2)
C(37)	−0·2182 (8)	0·3538 (5)	0·140 (1)	4·6 (2)
C(38)	−0·316 (1)	0·4062 (6)	0·146 (1)	5·7 (3)
C(39)	−0·4428 (8)	0·3816 (5)	0·0819 (8)	4·3 (2)
C(40)	−0·4692 (8)	0·3017 (6)	0·010 (1)	4·6 (2)
C(41)	−0·3727 (9)	0·2474 (6)	0·0034 (9)	4·7 (2)
C(42)	−0·549 (1)	0·4384 (7)	0·092 (1)	6·7 (3)
H(1)	0·021	0·169	0·306	3·9*

The starred atom was refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: $(8\pi^2/3)[U_{11}a^2a^{*2} + U_{22}b^2b^{*2} + U_{33}c^2c^{*2} + 2U_{12}aba^*b^*\cos\gamma + \cdots]$.

Table 2. *Distances (Å) and angles (°) with e.s.d.'s in parentheses*

Pt(1)—Cl(1)	2·384 (3)	C(17)—C(18)	1·38 (1)
Pt(1)—P(1)	2·278 (2)	C(18)—C(19)	1·37 (2)
Pt(1)—P(2)	2·282 (2)	C(18)—C(21)	1·49 (2)
P(1)—C(22)	1·837 (9)	C(19)—C(20)	1·40 (2)
P(1)—C(29)	1·822 (9)	C(22)—C(23)	1·38 (1)
P(1)—C(36)	1·802 (9)	C(22)—C(27)	1·39 (1)
P(2)—C(1)	1·820 (8)	C(23)—C(24)	1·39 (1)
P(2)—C(8)	1·819 (8)	C(24)—C(25)	1·38 (2)
P(2)—C(15)	1·817 (9)	C(25)—C(26)	1·35 (1)
C(1)—C(2)	1·39 (1)	C(25)—C(28)	1·50 (1)
C(1)—C(6)	1·39 (1)	C(26)—C(27)	1·38 (1)
C(2)—C(3)	1·39 (1)	C(29)—C(30)	1·36 (1)
C(3)—C(4)	1·35 (1)	C(29)—C(34)	1·37 (1)
C(4)—C(5)	1·40 (1)	C(30)—C(31)	1·40 (1)
C(4)—C(7)	1·52 (2)	C(31)—C(32)	1·35 (1)
C(5)—C(6)	1·38 (1)	C(32)—C(33)	1·38 (2)
C(8)—C(9)	1·40 (1)	C(32)—C(35)	1·50 (2)
C(8)—C(13)	1·38 (1)	C(33)—C(34)	1·38 (1)
C(9)—C(10)	1·38 (1)	C(36)—C(37)	1·42 (1)
C(10)—C(11)	1·39 (1)	C(36)—C(41)	1·38 (1)
C(11)—C(12)	1·35 (1)	C(37)—C(38)	1·38 (1)
C(11)—C(14)	1·51 (1)	C(38)—C(39)	1·37 (1)
C(12)—C(13)	1·40 (1)	C(39)—C(40)	1·37 (1)
C(15)—C(16)	1·40 (1)	C(39)—C(42)	1·50 (1)
C(15)—C(20)	1·38 (1)	C(40)—C(41)	1·38 (1)
C(16)—C(17)	1·38 (1)		

Cl(1)—Pt(1)—P(1)	94·52 (8)	C(15)—C(16)—C(17)	120·5 (7)
Cl(1)—Pt(1)—P(2)	97·98 (8)	C(16)—C(17)—C(18)	122 (1)
P(1)—Pt(1)—P(2)	167·18 (9)	C(17)—C(18)—C(19)	117 (1)
Pt(1)—P(1)—C(22)	113·9 (2)	C(17)—C(18)—C(21)	122 (1)
Pt(1)—P(1)—C(29)	117·3 (3)	C(19)—C(18)—C(21)	120·9 (9)
Pt(1)—P(1)—C(36)	113·1 (2)	C(18)—C(19)—C(20)	122·4 (9)
C(22)—P(1)—C(29)	103·5 (4)	C(15)—C(20)—C(19)	120 (1)
C(22)—P(1)—C(36)	102·9 (4)	P(1)—C(22)—C(23)	124·1 (8)
C(29)—P(1)—C(36)	104·6 (4)	P(1)—C(22)—C(27)	118·0 (6)
Pt(1)—P(2)—C(1)	109·8 (2)	C(23)—C(22)—C(27)	117·9 (8)
Pt(1)—P(2)—C(8)	114·7 (2)	C(22)—C(23)—C(24)	121 (1)
Pt(1)—P(2)—C(15)	118·3 (3)	C(23)—C(24)—C(25)	121·6 (8)
C(1)—P(2)—C(8)	105·0 (4)	C(24)—C(25)—C(26)	116·5 (9)
C(1)—P(2)—C(15)	104·2 (3)	C(24)—C(25)—C(28)	121·3 (8)
C(8)—P(2)—C(15)	103·5 (4)	C(26)—C(25)—C(28)	122 (1)
P(2)—C(1)—C(2)	123·7 (6)	C(25)—C(26)—C(27)	124 (1)
P(2)—C(1)—C(6)	117·5 (7)	C(22)—C(27)—C(26)	119·5 (8)
C(2)—C(1)—C(6)	118·7 (8)	P(1)—C(29)—C(30)	117·9 (6)
C(1)—C(2)—C(3)	120·1 (8)	P(1)—C(29)—C(34)	123·4 (7)
C(2)—C(3)—C(4)	121·8 (9)	C(30)—C(29)—C(34)	118·7 (8)
C(3)—C(4)—C(5)	118·5 (8)	C(29)—C(30)—C(31)	120·1 (8)
C(3)—C(4)—C(7)	119·3 (9)	C(30)—C(31)—C(32)	122 (1)
C(5)—C(4)—C(7)	122·1 (9)	C(31)—C(32)—C(33)	118 (1)
C(4)—C(5)—C(6)	120·6 (7)	C(31)—C(32)—C(35)	122 (1)
C(1)—C(6)—C(5)	120·3 (8)	C(33)—C(32)—C(35)	119·6 (9)
P(2)—C(8)—C(9)	121·1 (6)	C(32)—C(33)—C(34)	120·6 (9)
P(2)—C(8)—C(13)	121·1 (5)	C(29)—C(34)—C(33)	120·8 (9)
C(9)—C(8)—C(13)	117·8 (7)	P(1)—C(36)—C(37)	120·7 (6)
C(8)—C(9)—C(10)	120·6 (8)	P(1)—C(36)—C(41)	123·3 (6)
C(9)—C(10)—C(11)	121·5 (7)	C(37)—C(36)—C(41)	116·0 (8)
C(10)—C(11)—C(12)	117·5 (9)	C(36)—C(37)—C(38)	121·1 (8)
C(10)—C(11)—C(14)	121·9 (7)	C(37)—C(38)—C(39)	122·0 (8)
C(12)—C(11)—C(14)	120·6 (8)	C(38)—C(39)—C(40)	117·4 (9)
C(11)—C(12)—C(13)	122·7 (8)	C(38)—C(39)—C(42)	121·7 (8)
C(8)—C(13)—C(12)	120·0 (7)	C(40)—C(39)—C(42)	120·8 (8)
P(2)—C(15)—C(16)	118·7 (5)	C(39)—C(40)—C(41)	121·9 (8)
P(2)—C(15)—C(20)	123·7 (8)	C(36)—C(41)—C(40)	121·7 (8)
C(16)—C(15)—C(20)	117·6 (9)		

and -0.96 e Å^{-3}, e.s.d. of observations of unit weight $= 1.05$, atomic scattering factors for neutral Pt, P, Cl, C and H atoms, and values of f' and f'' for all non-H atoms from *International Tables for X-ray Crystallography* (1974); computer programs *SDP*/VAX (Frenz, 1978)

Discussion. Final atomic coordinates for non-H atoms are listed in Table 1 and principal bond lengths and angles are listed in Table 2.* The atom-numbering scheme is shown in Fig. 1.

The geometry about the Pt center in (2) is distorted square planar with the chloride ligand mutually *cis* to the two P donor atoms. The hydride ligand (not located in the difference map) is assumed to occupy the site *trans* to Cl(1). A comparison of key bond lengths and angles with those found in three other *trans*-[PtH(Cl)(PR₃)₂] complexes is shown in Table 3, along with the values of the Tolman cone angles (Tolman, 1977) of each of the tertiary phosphine ligands. Evident from the data in Tables 2 and

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* Lists of structure factors, anisotropic thermal parameters and calculated hydrogen positions have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52163 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
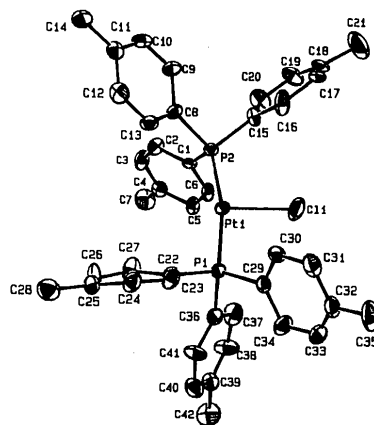

Fig. 1. *ORTEP* (Johnson, 1965) drawing showing the atom-numbering scheme and 50% probability ellipsoids.

Table 3. *Selected bond lengths (Å) and angles (°) of trans-[Pt(Cl)(H)(PR₃)₂] complexes*

Ligand	Pt—Cl(1)	Pt—P(1)	Pt—P(2)	P(2)—Pt—Cl(1)	P(1)—Pt—Cl(1)	P(1)—Pt—P(2)	Tolman cone angle	Reference
P(tolyl)₃	2·384 (3)	2·278 (2)	2·282 (2)	97·98 (8)	94·52 (8)	167·18 (9)	145	This work
PPh₂Et	2·422 (9)	2·267 (8)	2·269 (8)	94·5 (4)	92·6 (4)	171·2 (3)	140	Eisenberg & Ibers (1965)
PMe₃	2·423 (6)	2·280 (6)	2·281 (6)	—	—	176·0 (2)	118	Packett, Jensen, Cowan, Strouse & Trogler (1985)
PPh₃	2·36 (1)	2·30 (1)	2·15 (2)	91 (1)	93 (1)	173 (1)	145	Bender, Braunstein, Jud & Dusausory (1984)

3 is the bending of the tertiary phosphine ligands away from the chloride site and towards the hydride site. This distortion from linearity of the P—Pt—P axis might be expected to correlate with the steric bulk of the PR_3 ligands. Inspection of Table 3 shows that the $\angle$P—Pt—P is closest to 180° with the smallest ligand (PMe$_3$). The Pt—Cl(1) distance in (2) is similar to that found in (1) (Table 3), indicating little difference in *cis*-influence for the PPh$_3$ and P(*p*-tolyl)$_3$ ligands.

The geometry of the P(*p*-tolyl)$_3$ ligands in (2) is unexceptional and the bond lengths and angles associated with this ligand are comparable with those found in other P(*p*-tolyl)$_3$ complexes of platinum-group metals (Kaduk & Ibers, 1977).

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Structures of Two Isomorphous Fe—Phosphine Complexes. II. (η-C$_5$H$_5$)Fe(CO)(COMe)(PPh$_3$) (1) and (η-MeC$_5$H$_4$)Fe(CO)(COMe)(PPh$_3$) (2)

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Abstract. The complexes are monoclinic, $P2_1/c$, λ(Mo $K\alpha$) = 0·71073 Å, T = 293 K. (1) Acetyl(carbonyl)(η^5-cyclopentadienyl)(triphenylphosphine)-iron, [Fe(C$_2$H$_3$O)(C$_5$H$_5$)(CO){P(C$_6$H$_5$)$_3$}], M_r = 454·29, a = 7·903 (3), b = 15·884 (6), c = 17·763 (6) Å, β = 96·21 (4)°, V = 2216·7 (1·7) Å^3, Z = 4, D_x = 1·361, D_m = 1·38 g cm^{-3}, μ = 7·7 cm^{-1}, $F(000)$ = 944, $R(F)$ = 0·061, wR = 0·048 for 1992 reflections with $F_o > 3\sigma(F_o)$. (2) Acetyl(carbonyl)(η^5-methylcyclopentadienyl)(triphenylphosphine)iron, [Fe(C$_2$H$_3$O)(C$_6$H$_7$)(CO){P(C$_6$H$_5$)$_3$}], M_r = 468·32, a = 7·873 (2), b = 16·018 (6), c = 18·048 (7) Å, β = 96·15 (3)°, V = 2262·9 (1·3) Å^3, Z = 4, D_x = 1·374, D_m = 1·36 g cm^{-3}, μ = 7·6 cm^{-1}, $F(000)$ = 976, $R(F)$ = 0·065, wR = 0·047 for 1769 reflections with $F_o > 3\sigma(F_o)$. The Fe—P bond length is 2·202 (2) Å for (1) and 2·195 (2) Å for (2), and the torsion angles O(2)—C(2)—Fe—(CO) [C(2) = acetyl carbon] are 18 (*anti*) and 22° (*anti*), respectively. In both structures the Fe atom is located centrally above the five-membered ring; Fe—ring-center 1·752 (5) and 1·746 (8) Å for (1) and (2) respectively.

Introduction. Complexes of the type (η-C$_5$H$_5$)-Fe(CO)(COMe)L and (η-MeC$_5$H$_4$)Fe(CO)(COMe)L where L is a phosphine ligand are very useful in our studies of quantitative analysis of ligand effects (QALE) (Rahman, Liu, Eriks, Prock & Giering, 1989). The QALE model allows one to separate σ and π effects in the Fe—L bond and, more generally, it postulates that electronic and steric ligand effects are separable. Furthermore, the model leads to the conclusion that the Fe—P bond distance is a good diagnostic of σ-bonded or π-bonded phosphine ligands. The abrupt onset of steric effects (steric threshold) for σ-donor ligands suggests that

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