Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^4$)

$U_{eq} = \frac{1}{3}$ (trace of the orthogonalized U_{ij} matrix).

	x	*y*	*z*	U_{eq}
Pd	5000	5000	5000	353 (1)
Cl	6334 (1)	6546 (1)	4313 (1)	644 (3)
N	3000 (2)	5614 (2)	4020 (2)	387 (7)
C(1)	2726 (3)	5285 (2)	2528 (3)	415 (9)
C(2)	1861 (3)	4350 (3)	2187 (3)	579 (11)
C(3)	1603 (4)	4036 (3)	752 (4)	664 (13)
C(4)	2235 (4)	4625 (3)	−320 (4)	708 (13)
C(5)	3083 (6)	5540 (4)	34 (4)	973 (18)
C(6)	3358 (5)	5874 (3)	1461 (3)	775 (14)
C(7)	2032 (3)	6230 (2)	4626 (3)	469 (9)
C(8)	2321 (4)	6519 (3)	6196 (3)	624 (12)
C(9)	590 (4)	6705 (3)	3850 (4)	712 (13)

Table 2. *Bond lengths* (Å) *and angles* (°)

Pd–Cl	2·303 (1)	Pd–N	2·024 (2)
N–C(1)	1·439 (4)	N–C(7)	1·273 (4)
C(1)–C(2)	1·377 (4)	C(1)–C(6)	1·360 (5)
C(2)–C(3)	1·384 (5)	C(3)–C(4)	1·363 (5)
C(4)–C(5)	1·351 (6)	C(5)–C(6)	1·385 (5)
C(7)–C(8)	1·497 (4)	C(7)–C(9)	1·499 (4)
Cl–Pd–N	89·9 (1)	Pd–N–C(1)	113·9 (2)
Pd–N–C(7)	125·1 (2)	C(1)–N–C(7)	121·1 (2)
N–C(1)–C(2)	119·8 (3)	N–C(1)–C(6)	120·2 (3)
C(2)–C(1)–C(6)	119·9 (3)	C(1)–C(2)–C(3)	119·6 (3)
C(2)–C(3)–C(4)	120·5 (3)	C(3)–C(4)–C(5)	119·1 (3)
C(4)–C(5)–C(6)	121·6 (4)	C(1)–C(6)–C(5)	119·2 (3)
N–C(7)–C(8)	119·6 (3)	N–C(7)–C(9)	123·5 (3)
C(8)–C(7)–C(9)	116·8 (3)		

ordinates and U_{eq} values for the non-hydrogen atoms, and Table 2 lists selected bond lengths and angles.*

Related literature. Similar square-planar Pd complexes with related ligands have been reported by Anderson & Einstein (1978), Einstein & Field (1979), Keijsper, van der Poel, Polm, van Koten, Vrieze, Seignette, Varenhorst & Stam (1983) and, most closely related, Kuz'mina & Struchkov (1979).

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43733 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of (Benzylideneacetone)tricarbonyliron (Monoclinic Form)

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Abstract. Tricarbonyl(η^4-1-phenyl-1-buten-3-one)-iron, $[Fe(CO)_3(C_{10}H_{10}O)]$, $M_r = 286{\cdot}05$, monoclinic, $P2_1/a$, $a = 10{\cdot}4439$ (16), $b = 12{\cdot}7485$ (23), $c = 10{\cdot}6642$ (16) Å, $\beta = 116{\cdot}330$ (13)°, $V = 1272{\cdot}6$ Å^3, $Z = 4$, $D_x = 1{\cdot}493$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 11{\cdot}84$ cm^{-1}, $F(000) = 584$, room temperature, final $R = 0{\cdot}0255$ for 1869 independent observed reflections. The molecular structure is essentially the same as that in the orthorhombic form [Hubener, Kuhr & Weiss (1981). *Cryst. Struct. Commun.* **10**, 1451–1455]. The phenyl group makes an angle of 24 (1)° to the rest of the ligand.

Experimental. Crystallization by cooling a solution (hexane:CH_2Cl_2, 10:1) gave needles (*Pbca*) and plates; yellow plate 0·3 × 0·3 × 0·1 mm selected; D_m not measured. Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation; lattice parameters from refinement of 25 reflections in range $10{\cdot}7 < \theta < 13{\cdot}7°$; 4739 reflection intensities measured by $\omega/2\theta$ scan, scan width 0·8° +0·35° tanθ, θ 1→25°, h −12→12, k 0→15, l 0→12 and some equivalents. Empirical absorption correction 0·906–1·167; correction for decay of two standard reflections by about 15%. 2241 unique reflections, $R_{int} = 0{\cdot}016$, 1869 with

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Table 1. *Fractional coordinates and equivalent isotropic thermal parameters of atoms*

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij} a_i^* a_i^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq} (Å^2)
Fe(1)	0·44058 (3)	0·29088 (2)	0·11734 (3)	0·0399 (2)
O(1)	0·39974 (16)	0·19812 (11)	0·24850 (17)	0·0558 (10)
C(1)	0·6005 (3)	0·08165 (21)	0·2924 (3)	0·0624 (19)
C(2)	0·53606 (23)	0·18803 (16)	0·28285 (22)	0·0472 (14)
C(3)	0·61327 (23)	0·28293 (17)	0·31161 (20)	0·0428 (12)
C(4)	0·53750 (23)	0·37574 (17)	0·30891 (21)	0·0463 (14)
C(5)	0·59569 (22)	0·48283 (16)	0·32345 (20)	0·0443 (13)
C(6)	0·7179 (3)	0·50568 (18)	0·30686 (23)	0·0549 (16)
C(7)	0·7676 (3)	0·60800 (20)	0·3212 (3)	0·0673 (19)
C(8)	0·6989 (3)	0·68766 (20)	0·3531 (3)	0·0703 (20)
C(9)	0·5802 (4)	0·66556 (21)	0·3705 (3)	0·0705 (20)
C(10)	0·5279 (3)	0·56500 (19)	0·35532 (23)	0·0562 (16)
C(20)	0·28033 (24)	0·37081 (18)	0·04356 (24)	0·0532 (15)
O(20)	0·17981 (20)	0·41935 (15)	−0·00591 (22)	0·0816 (14)
C(30)	0·39033 (24)	0·18978 (17)	−0·01612 (24)	0·0511 (15)
O(30)	0·35552 (21)	0·12939 (14)	−0·10314 (19)	0·0752 (13)
C(40)	0·53364 (22)	0·35715 (16)	0·03703 (21)	0·0451 (13)
O(40)	0·59585 (17)	0·39882 (13)	−0·01314 (17)	0·0653 (12)
H(11)	0·605 (3)	0·0528 (24)	0·363 (3)	0·083 (10)
H(12)	0·538 (3)	0·0355 (22)	0·215 (3)	0·0807 (87)
H(13)	0·690 (4)	0·0859 (25)	0·283 (3)	0·107 (12)
H(3)	0·6996 (22)	0·2813 (14)	0·3183 (20)	0·0350 (52)
H(4)	0·4662 (25)	0·3702 (17)	0·3383 (23)	0·0521 (62)
H(6)	0·768 (3)	0·4502 (20)	0·289 (3)	0·0659 (74)
H(7)	0·857 (3)	0·6188 (20)	0·319 (3)	0·0676 (77)
H(8)	0·739 (3)	0·7636 (21)	0·360 (3)	0·0731 (75)
H(9)	0·536 (3)	0·7164 (20)	0·389 (3)	0·0702 (88)
H(10)	0·444 (3)	0·5509 (17)	0·3662 (23)	0·0555 (67)

Table 2. *Bond lengths* (Å) *and selected angles* (°)

O(1)–C(2)	1·310 (3)	C(6)–H(6)	0·95 (3)
C(1)–C(2)	1·497 (4)	C(7)–H(7)	0·96 (3)
C(2)–C(3)	1·410 (3)	C(8)–H(8)	1·05 (3)
C(3)–C(4)	1·417 (3)	C(9)–H(9)	0·87 (3)
C(4)–C(5)	1·474 (3)	C(10)–H(10)	0·946 (25)
C(5)–C(6)	1·394 (3)	Fe(1)–O(1)	2·0164 (17)
C(5)–C(10)	1·388 (3)	Fe(1)–C(2)	2·0658 (23)
C(6)–C(7)	1·387 (4)	Fe(1)–C(3)	2·0593 (23)
C(7)–C(8)	1·371 (4)	Fe(1)–C(4)	2·1294 (23)
C(8)–C(9)	1·362 (4)	Fe(1)–C(20)	1·8139 (25)
C(9)–C(10)	1·375 (4)	Fe(1)–C(30)	1·8165 (24)
C(1)–H(11)	0·82 (3)	Fe(1)–C(40)	1·7693 (22)
C(1)–H(12)	0·99 (3)	C(20)–O(20)	1·128 (3)
C(1)–H(13)	0·99 (4)	C(30)–O(30)	1·134 (3)
C(3)–H(3)	0·873 (21)	C(40)–O(40)	1·140 (3)
C(4)–H(4)	0·930 (24)		

O(1)–Fe(1)–C(2)	37·40 (8)	C(6)–C(5)–C(10)	117·91 (21)
O(1)–Fe(1)–C(3)	68·51 (8)	C(5)–C(6)–C(7)	120·09 (23)
O(1)–Fe(1)–C(4)	77·83 (8)	C(6)–C(7)–C(8)	120·8 (3)
C(2)–Fe(1)–C(3)	39·98 (9)	C(7)–C(8)–C(9)	119·3 (3)
C(2)–Fe(1)–C(4)	70·05 (9)	C(8)–C(9)–C(10)	121·0 (3)
C(3)–Fe(1)–C(4)	39·49 (9)	C(5)–C(10)–C(9)	120·90 (25)
O(1)–C(2)–C(1)	120·55 (22)	C(20)–Fe(1)–C(30)	99·69 (11)
O(1)–C(2)–C(3)	114·99 (20)	C(20)–Fe(1)–C(40)	96·95 (11)
C(1)–C(2)–C(3)	124·46 (22)	C(30)–Fe(1)–C(40)	89·39 (11)
C(2)–C(3)–C(4)	116·86 (20)	Fe(1)–C(20)–O(20)	178·06 (23)
C(3)–C(4)–C(5)	124·81 (20)	Fe(1)–C(30)–O(30)	177·33 (22)
C(4)–C(5)–C(6)	122·53 (20)	Fe(1)–C(40)–O(40)	178·71 (20)
C(4)–C(5)–C(10)	119·56 (20)		

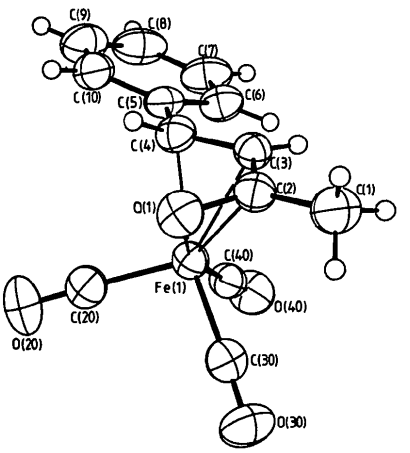

Fig. 1. Perspective view of (benzylideneacetone)tricarbonyliron. Thermal ellipsoids at 50% probability level, except for H atoms which are given a fixed radius for clarity.

$F > 2\sigma(F)$. Structure solved from Patterson and difference syntheses, structure refined by full-matrix least squares on F. Anisotropic thermal parameters for all non-H atoms, H atoms refined with isotropic thermal parameters, $R = 0{\cdot}0255$, $wR = 0{\cdot}0296$, $S = 1{\cdot}420$, $w^{-1} = \sigma^2(F) + gF^2$, g refined to 0·000223, $(\Delta/\sigma)_{max} = 0{\cdot}069$, $\Delta\rho_{max} = 0{\cdot}212$, $\Delta\rho_{min} = -0{\cdot}198$ e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974). Programs: *SHELX*76 (Sheldrick, 1976), *DIFABS* (Walker & Stuart, 1983), *CALC* (Gould & Taylor, 1986), *EASYORTEP* (Mallinson, 1979). Table 1* gives the atom parameters and Table 2 bond lengths and angles. Fig. 1 shows the atomic numbering.

* Lists of structure factors, anisotropic thermal parameters and a full list of bond angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43718 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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