in Table 2.* Fig. 1 shows a molecular diagram and Fig. 2 the unit-cell contents.

Related literature. The structures of relatively few uranyl complexes which contain a U—N bond are known. They include the following pyridine diketonate complexes: $UO_2(CH_3COCHCOCH_3)_2C_5H_5N$ (Alcock, Flanders & Brown, 1984a,b), UO_2-$(C_8H_{12}N)(CH_3COCHCH_3)_2$ (Alcock & Flanders, 1987), $UO_2(PhCOCHCOPh)_2(C_5H_5N)$ and UO_2-$(CH_3COCHCOOBu^t)_2(C_5H_5N)$ (Alcock, Flanders, Pennington & Brown, 1987), and have a range of U—N distances of 2·47 (1)–2·595 (2) Å. These distances are slightly shorter than in the bis-tropolonato uranyl

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, full bond lengths and angles, and details of mean planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51005 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

complex described by Degetto (U—N 2·62 Å; Degetto, Marangoni, Bombieri, Forsellini, Baracco & Gaziani, 1974).

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Structure of Benzoylferrocene

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Abstract. $(C_5H_5)Fe(C_5H_4COC_6H_5)$, $C_{17}H_{14}FeO$, M_r = 290·15, monoclinic, $P2_1/n$, $a = 6·1969$ (4), $b = 15·2293$ (3), $c = 13·9109$ (7) Å, $\beta = 99·180$ (3)°, $V = 1296·0$ (1) Å^3, $Z = 4$, $D_x = 1·487$ g cm^{-3}, $\lambda(\text{Mo }K\alpha_1) = 0·70930$ Å, $\mu = 11·3$ cm^{-1}, $F(000) = 600$, $T = 295$ K, $R = 0·028$ for 2310 reflections. The ferrocene group is 6° from an eclipsed orientation, with Fe—C = 2·035–2·053 (2), mean 2·043 Å (libration corrections increase all bond distances by ~0·01 Å). The C—C bonds in the substituted cyclopentadienyl (Cp) ring show evidence of some double-bond localization, with the bonds at the substituted C atom being 1·438 and 1·442 (3) Å, with the other three bonds 1·405, 1·421 and 1·411 (3) Å; in the other Cp ring, the C—C bonds are all in the range 1·405–1·411 (4) Å. The effect of this bond localization is also noted in the short Cp—CO distance of 1·467 (3) Å, relative to Ph—CO of 1·496 (3) Å. The carbonyl group is slightly non-planar [with the C atom 0·009 (2) Å out of the plane of the three bonded atoms and 0·040 (2) Å out of the Cp plane], and rotated 14·2° out of the Cp plane;

the phenyl group is rotated out of the carbonyl plane by a further 26·2°, these deviations from coplanarity being a result of steric interaction between Cp and Ph hydrogen atoms.

Experimental. Reaction of bis(benzonitrile)dichloropalladium with lithioferrocene gave a product which crystallized from dichloromethane/hexane as red wedges, {100}, (010), (001), (0$\bar{1}$2) developed, 0·18 × 0·25 × 0·27 mm. Enraf–Nonius CAD-4F diffractometer, lattice parameters from 25 reflections with $\theta = 20$–24°. Intensities for $\theta \le 30·0°$, hkl: 0 to 8, 0 to 21, −19 to 19, ω–2θ scan, ω scan width (0·60 + 0·35 tanθ)° at 1·3–10° min^{-1}, extended 25% on each side for background measurement, three standard reflections showed negligible variations in intensity, Lp and absorption corrections (numerical integration, transmission factors 0·664–0·836), 3764 independent reflections measured, 2310 with $I \ge 3\sigma(I)$, where $\sigma^2(I) = S + 4(B_1 + B_2) + (0·04I)^2$, S = scan, B_1 and B_2 = background counts. Structure by Patterson and

Table 1. *Positional (fractional) and equivalent isotropic thermal parameters* $(U_{eq}, \text{Å}^2)$

$$U_{eq} = \tfrac{1}{3}\sum_i\sum_j U_{ij}a_i^* a_j^* a_i . a_j .$$

	x	y	z	U_{eq}
Fe	0·37710 (4)	0·54033 (2)	0·23297 (2)	0·032
O	0·81908 (25)	0·36854 (15)	0·18428 (17)	0·077
C(1)	0·53686 (30)	0·42343 (13)	0·25810 (14)	0·033
C(2)	0·66258 (35)	0·49318 (14)	0·30939 (16)	0·040
C(3)	0·53777 (38)	0·53241 (14)	0·37366 (15)	0·044
C(4)	0·33379 (38)	0·48807 (14)	0·36403 (15)	0·040
C(5)	0·33037 (32)	0·42143 (14)	0·29330 (14)	0·035
C(6)	0·30137 (46)	0·56215 (16)	0·08627 (17)	0·052
C(7)	0·44534 (48)	0·62777 (18)	0·13002 (20)	0·062
C(8)	0·34367 (54)	0·67082 (16)	0·20045 (21)	0·063
C(9)	0·13749 (48)	0·63181 (17)	0·19969 (19)	0·057
C(10)	0·11123 (41)	0·56461 (17)	0·12930 (18)	0·051
C(11)	0·62262 (32)	0·36731 (13)	0·18718 (16)	0·041
C(12)	0·48092 (31)	0·30698 (13)	0·11949 (14)	0·034
C(13)	0·57870 (39)	0·23409 (15)	0·08487 (18)	0·046
C(14)	0·46054 (48)	0·17832 (17)	0·01888 (20)	0·057
C(15)	0·24207 (45)	0·19429 (16)	−0·01380 (17)	0·053
C(16)	0·14321 (38)	0·26612 (15)	0·01945 (16)	0·044
C(17)	0·26011 (33)	0·32246 (14)	0·08644 (15)	0·037

Fig. 1. Stereoview of the benzoylferrocene molecule.

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

Fe—C(1)	2·040 (2)	C(3)—C(4)	1·421 (3)
Fe—C(2)	2·043 (2)	C(4)—C(5)	1·411 (3)
Fe—C(3)	2·053 (2)	C(6)—C(7)	1·411 (4)
Fe—C(4)	2·046 (2)	C(6)—C(10)	1·405 (4)
Fe—C(5)	2·036 (2)	C(7)—C(8)	1·408 (4)
Fe—C(6)	2·047 (2)	C(8)—C(9)	1·408 (4)
Fe—C(7)	2·048 (2)	C(9)—C(10)	1·408 (4)
Fe—C(8)	2·041 (2)	C(11)—C(12)	1·496 (3)
Fe—C(9)	2·035 (2)	C(12)—C(13)	1·387 (3)
Fe—C(10)	2·043 (2)	C(12)—C(17)	1·392 (3)
O—C(11)	1·225 (2)	C(13)—C(14)	1·373 (3)
C(1)—C(2)	1·438 (3)	C(14)—C(15)	1·379 (4)
C(1)—C(5)	1·442 (3)	C(15)—C(16)	1·370 (3)
C(1)—C(11)	1·467 (3)	C(16)—C(17)	1·383 (3)
C(2)—C(3)	1·405 (3)		

C(2)—C(1)—C(5)	106·7 (2)	O—C(11)—C(1)	118·8 (2)
C(2)—C(1)—C(11)	122·6 (2)	O—C(11)—C(12)	118·4 (2)
C(5)—C(1)—C(11)	130·7 (2)	C(1)—C(11)—C(12)	122·8 (2)
C(1)—C(2)—C(3)	108·7 (2)	C(11)—C(12)—C(13)	117·7 (2)
C(2)—C(3)—C(4)	108·0 (2)	C(11)—C(12)—C(17)	123·4 (2)
C(3)—C(4)—C(5)	108·8 (2)	C(13)—C(12)—C(17)	118·8 (2)
C(1)—C(5)—C(4)	107·8 (2)	C(12)—C(13)—C(14)	120·7 (2)
C(7)—C(6)—C(10)	108·2 (2)	C(13)—C(14)—C(15)	120·1 (2)
C(6)—C(7)—C(8)	107·9 (2)	C(14)—C(15)—C(16)	119·9 (2)
C(7)—C(8)—C(9)	107·7 (2)	C(15)—C(16)—C(17)	120·6 (2)
C(8)—C(9)—C(10)	108·4 (2)	C(12)—C(17)—C(16)	119·9 (2)
C(6)—C(10)—C(9)	107·7 (2)		

Fourier methods, refined by full-matrix least squares on F, H atoms from a difference map, $w = 1/\sigma^2(F)$, scattering factors and anomalous-dispersion corrections for Fe from *International Tables for X-ray Crystallography* (1974), locally written, or locally modified versions of standard computer programs (Rettig & Trotter, 1986), final $R = 0\cdot028$, $wR = 0\cdot035$ for 2310 reflections, $S = 1\cdot43$, 228 parameters (one
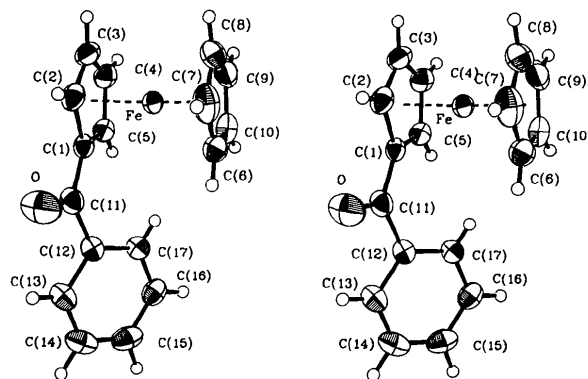
scale factor, 171 non-hydrogen-atom parameters, and 56 H-atom parameters), $R = 0\cdot072$ for all 3764 reflections, $\Delta/\sigma = 0\cdot10$ (mean), 0·6 [maximum, for B of H(9)], maximum final difference density $\pm0\cdot3$ e Å^{-3}. Atomic parameters are in Table 1, bond lengths and angles in Table 2, and a view of the molecule in Fig. 1.*

Related literature. Benzoylosmocene cell data (Macdonald & Trotter, 1965), diferrocenyl ketone (Trotter & Macdonald, 1966), dibenzoylferrocene (Struchkov & Khotsyanova, 1957), 1′-acetyl-1-benzoylferrocene (Calvarin & Weigel, 1971), phenylacetylferrocene (Gyepes & Hanic, 1975).

* Lists of anisotropic thermal parameters, H-atom positions, bond lengths and angles involving H, torsion angles, and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51034 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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