

$S = 1.082$
 5241 reflections
 246 parameters
 Only coordinates of H atoms refined
 $w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 3.3856P]$
 where $P = (F_o^2 + 2F_c^2)/3$

Extinction correction:
SHELXL93
 Extinction coefficient:
 0.0017 (3)
 Scattering factors from
International Tables for Crystallography (Vol. C)

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 Zsolnai, L. (1994). *XPMA. Program for Molecular Graphics*. University of Heidelberg, Germany.

Table 1. Selected geometric parameters (Å, °)

| | | | |
|------------|-----------|-------------|-----------|
| Ni1—N8 | 1.906 (3) | N1—C2 | 1.505 (5) |
| Ni1—N5 | 1.906 (3) | C4—N5 | 1.286 (5) |
| Ni1—N1 | 1.911 (3) | N8—C9 | 1.282 (6) |
| Ni1—N12 | 1.913 (4) | | |
| N8—Ni1—N5 | 86.6 (2) | C4—N5—C6 | 120.8 (4) |
| N8—Ni1—N1 | 173.3 (2) | C4—N5—Ni1 | 130.4 (3) |
| N5—Ni1—N1 | 93.5 (2) | C6—N5—Ni1 | 108.8 (3) |
| N8—Ni1—N12 | 91.9 (2) | C9—N8—C7 | 118.0 (4) |
| N5—Ni1—N12 | 178.4 (2) | C9—N8—Ni1 | 130.1 (3) |
| N1—Ni1—N12 | 88.0 (2) | C7—N8—Ni1 | 110.2 (3) |
| C2—N1—Ni1 | 120.2 (3) | N8—C9—C10 | 121.8 (4) |
| N5—C4—C3 | 120.6 (4) | C11—N12—Ni1 | 118.7 (3) |

Table 2. Hydrogen-bonding geometry (Å, °)

| D—H...A | D—H | H...A | D...A | D—H...A |
|------------------------------|----------|----------|-----------|---------|
| N1—H1A...C11 ⁱ | 0.92 (5) | 2.48 (5) | 3.401 (4) | 174 (4) |
| N1—H1B...C12 ⁱⁱ | 0.91 (5) | 2.50 (4) | 3.389 (4) | 167 (4) |
| N12—H12A...C11 ⁱ | 0.79 (5) | 2.64 (5) | 3.426 (4) | 177 (4) |
| N12—H12B...C14 ⁱⁱ | 0.83 (5) | 2.59 (4) | 3.306 (4) | 145 (4) |

Symmetry codes: (i) $x, -\frac{1}{2} - y, z - \frac{1}{2}$; (ii) $2 - x, y - \frac{1}{2}, \frac{1}{2} - z$.

Neutral atom-scattering factors were from Ibers & Hamilton (1992). Non-H atom parameters were refined anisotropically. Atoms H1A, H1B, H12A and H12B were located from difference maps, other H-atom positions were calculated and parameters were refined in isotropic approximation.

Data collection: *SMART* (Siemens, 1995). Cell refinement: local programs. Data reduction: *SAINT* (Siemens, 1995). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *XPMA* (Zsolnai, 1994). Software used to prepare material for publication: *SHELXL93*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1009). Services for accessing these data are described at the back of the journal.

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Accurate Redeterminations of 1,1'-Di-benzoylferrocene and (4-Nitrophenyl)-ferrocene

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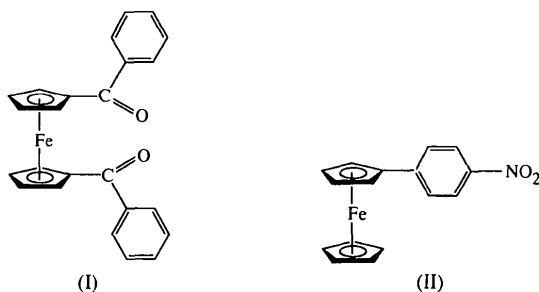
Abstract

In the solid state, molecules of 1,1'-dibenzoylferrocene, [Fe(C₁₂H₉O)₂], (I), are linked to form infinite chains in the [100] direction via (cyclopentadienyl)C—H...O hydrogen bonds [C...O 3.354 (4) Å]. In the structure of (4-nitrophenyl)ferrocene, [Fe(C₅H₅)(C₁₁H₈NO₂)], (II), there are no C—H...O hydrogen bonds and molecules are separated by normal van der Waals distances. For earlier determinations see Struchkov [*Dokl. Akad. Nauk SSSR* (1956), 110, 67–70] for (I) and Roberts *et al.* [*J. Chem. Soc. Dalton Trans.* (1988), pp. 1549–1556] for (II).

Comment

The structure of 1,1'-dibenzoylferrocene, [Fe(C₅H₄CO-Ph)₂], (I), was reported many years ago (Struchkov, 1956) and there are a number of reasons why this structure should be redetermined to modern standards. First, the unit cell was described as monoclinic ($P2_1/n$), but with $\beta = 90(1)^\circ$; secondly, there are no coordinate data for this compound in the Cambridge Structural Database (Allen & Kennard, 1993) or indeed in the original publication, although uncertainties on the C—C bond lengths are quoted, all in the range 0.03–0.05 Å (Struchkov, 1956); thirdly, the illustrations in the original report suggest the possibility that the molecules are close to having twofold rotational symmetry, and finally, the original report appeared long

before the possible occurrence of C—H...O hydrogen bonds in crystals had been envisaged. Since the analogous 1,2-diketones [Fe(C₅H₅)(C₅H₄COCOPh)] and [Fe(C₅H₄COCOPh)₂] both exhibit C—H...O hydrogen bonding (Glidewell *et al.*, 1996; Ferguson *et al.*, 1996), there is the possibility that the structure of (I) may also show such features. 1,1'-Dibenzoylferrocene is the archetypal diarylferrocene and it is an important compound in the ferrocene series: the lack of reliable structural data became apparent during a study of (1'-benzoylferrocenyl)diphenylmethanol, [(PhCOC₅H₄)Fe(C₅H₄CPh₂OH)] (Glidewell *et al.*, 1997), and accordingly we have now redetermined the structure of (I). We have also taken the opportunity to redetermine, to modern standards, the structure of (4-nitrophenyl)ferrocene [Fe(C₅H₅)(C₁₁H₈NO₂)] (II). The structure of (II) was originally refined (Roberts *et al.*, 1988) from two-circle data without any absorption correction to a rather high *R* value of 0.079, albeit for only 1149 observed data with $I > 2\sigma(I)$: the large s.u.'s on both the unit-cell parameters and the atom coordinates led to s.u.'s in the range 0.014–0.021 Å (average 0.017 Å) for bond lengths not involving iron, although s.u.'s on angles between least-squares planes were quoted as 0.1°.



The present structure determination for (I) confirms the space group as $P2_1/n$ with β of 90.060(8)°, as compared with the value of 90(1)° originally reported (Struchkov, 1956). The cell dimensions found here are rather smaller than those reported by Struchkov, $a = 11.69(2)$, $b = 25.36(5)$, $c = 6.27(1)$ Å, so that the unit-cell volume is *ca* 1.6% less than that given earlier (1859 Å³).

Within the molecules of (I), the corresponding bond lengths and angles in the two Fe(C₅H₄COPh) fragments are almost identical (Table 1), but any potential rotational symmetry is destroyed by the conformations of the phenyl rings. For example, the values of the torsional angles O1—C1—C11—C12 and O2—C2—C41—C42 would be identical in both magnitude and sign in the presence of a twofold rotation axis: the conformations of the two benzoyl groups actually observed are such that if they were both on the same cyclopentadienyl ring, the molecule would exhibit approximate mirror symmetry. The other conformational feature of importance is

the relative twist of the two C₅H₄COPh units: the most common conformation of 1,1'-disubstituted ferrocenes is eclipsed rings with the two exocyclic C—C bonds offset by one fifth of a rotation. In compound (I), the mean value of the torsion angle C1_{*n*}—Cg1—Cg2—C2_{*n*} ($n = 1-5$; Cg1 and Cg2 are the centroids of the two cyclopentadienyl rings) is 134.8(2)°, corresponding to nearly eclipsed rings, but with the exocyclic C—C bonds offset by two fifths of a turn: a mean value of $(n \times 72)^\circ$ ($n = 0$ or integer) represents complete eclipsing of the rings. The molecules therefore have no symmetry in the solid state and are thus chiral: the space group accommodates equal numbers of the two enantiomers. In solution, essentially free rotation about single C—C bonds, and of the two cyclopentadienyl rings relative to one another, accounts for the very simple NMR spectra. The angle between the best planes through the cyclopentadienyl rings is 0.5(2)°, and the Cg1—Fe—Cg2 angle is 179.4(3)°.

Although the two O atoms in (I) are both potential acceptors of C—H...O hydrogen bonds, only O2 acts in this manner. Atom C14 (Fig. 1) in the molecule at (x, y, z) acts as donor to atom O2 in the molecule at $(1+x, y, z)$, so generating a chain running parallel to the [100] direction in which the hydrogen-bonding motif has graph set $C(6)$ (Etter, 1990; Bernstein *et al.*, 1995). This chain is generated by translation whereas in [Fe(C₅H₅)(C₅H₄COCOPh)], $C(6)$ chains are generated by the action of a 2₁ axis (Glidewell *et al.*, 1996).

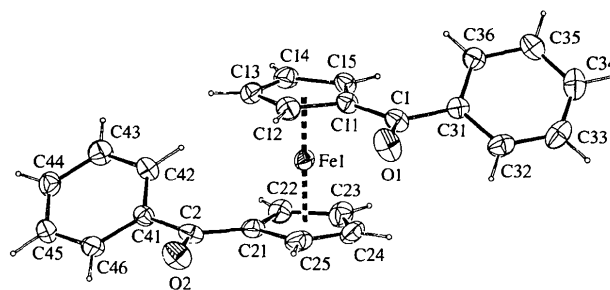


Fig. 1. A view of (I) showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

The refinement for (II) reproduces the general features described earlier (Roberts *et al.*, 1988) but with a much higher precision, giving a much smaller *R* value for significantly more observed data. The s.u.'s on the cell dimensions are about one sixth of those originally reported, and those on bond lengths and angles are typically less than one third of those cited earlier. The conformation of the ferrocenyl unit is almost eclipsed, as judged by the mean value of 6.7(3)° for the C1_{*n*}—Cg1—Cg2—C2_{*n*} ($n = 1-5$) torsion angle: the angle between the best planes through the cyclopentadienyl rings is 0.6(2)°, and the Cg1—Fe—Cg2

angle is 179.3(3)°. The angles between the planes defined by C11–C15 and C31–C36, and between C31–C36 and the CNO₂ fragment are 12.7(2)° and 2.7(3)°, respectively. Although the nitro group is well established as a powerful acceptor of C—H...O hydrogen bonds (Biradha *et al.*, 1993; Sharma & Desiraju, 1994), there are no intermolecular contacts in (II) less than the sum of the van der Waals radii: in particular, there are no C—H...O hydrogen bonds.

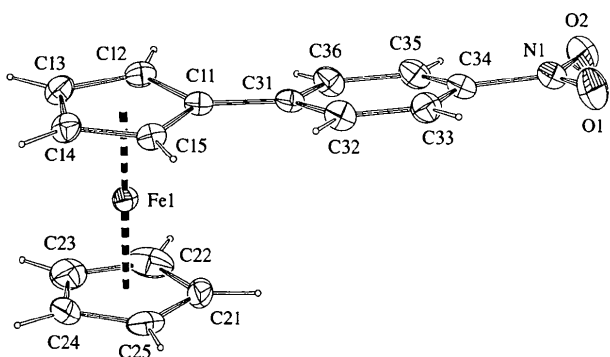


Fig. 2. A view of (II) showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 20% probability level.

Experimental

A sample of (I) was prepared by standard Friedel–Crafts acylation of ferrocene using PhCOCl/AlCl₃ in CH₂Cl₂ solution; a sample of (II) was prepared by reaction of ferrocene with a freshly diazotized solution of 4-nitroaniline in dilute sulfuric acid, followed by chromatography on alumina, using CH₂Cl₂–light petroleum (b.p. 313–333 K) as eluent. Crystals of (I) and (II) suitable for single-crystal X-ray diffraction were grown by slow evaporation of solutions in light petroleum and ethanol–CH₂Cl₂, respectively.

Compound (I)

Crystal data

| | |
|--|---|
| [Fe(C ₁₂ H ₉ O) ₂] | Mo K α radiation |
| $M_r = 394.23$ | $\lambda = 0.7107 \text{ \AA}$ |
| Monoclinic | Cell parameters from 25 reflections |
| $P2_1/n$ | $\theta = 9.42\text{--}22.43^\circ$ |
| $a = 6.2616(8) \text{ \AA}$ | $\mu = 0.840 \text{ mm}^{-1}$ |
| $b = 25.1866(15) \text{ \AA}$ | $T = 294(1) \text{ K}$ |
| $c = 11.6030(9) \text{ \AA}$ | Needle |
| $\beta = 90.060(8)^\circ$ | $0.44 \times 0.13 \times 0.09 \text{ mm}$ |
| $V = 1829.9(3) \text{ \AA}^3$ | Red |
| $Z = 4$ | |
| $D_x = 1.431 \text{ Mg m}^{-3}$ | |
| D_m not measured | |

Data collection

| | |
|-----------------------------------|--|
| Enraf–Nonius CAD-4 diffractometer | 2415 reflections with $I > 2\sigma(I)$ |
| ω – 2θ scans | $R_{\text{int}} = 0.009$ |

Absorption correction: empirical, 5 ψ scans at 4° steps (North, Phillips & Mathews, 1968)
 $T_{\text{min}} = 0.780$, $T_{\text{max}} = 0.816$
 4639 measured reflections
 4171 independent reflections

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.088$
 $S = 0.996$
 4171 reflections
 244 parameters
 H atoms constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.1903P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$\theta_{\text{max}} = 27.4^\circ$
 $h = -8 \rightarrow 8$
 $k = 0 \rightarrow 32$
 $l = 0 \rightarrow 15$
 3 standard reflections
 frequency: 120 min
 intensity variation: 1%

$(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.280 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.242 \text{ e \AA}^{-3}$
 Extinction correction: none
 Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. Selected geometric parameters (\AA , $^\circ$) for (I)

| | | | |
|-----------------|-----------|---------------|-----------|
| Fe1–Cg1† | 1.646(2) | C1–C11 | 1.476(3) |
| Fe1–Cg2 | 1.650(2) | C1–C31 | 1.489(4) |
| O1–C1 | 1.222(3) | C2–C21 | 1.476(4) |
| O2–C2 | 1.222(3) | C2–C41 | 1.490(4) |
| O1–C1–C11 | 118.9(3) | O2–C2–C21 | 119.4(3) |
| O1–C1–C31 | 119.5(2) | O2–C2–C41 | 118.6(3) |
| C11–C1–C31 | 121.6(2) | C21–C2–C41 | 122.0(2) |
| C11–Cg1–Cg2–C21 | 134.6(2) | O2–C2–C21–C22 | 172.0(3) |
| C12–Cg1–Cg2–C22 | 135.0(2) | O2–C2–C21–C25 | –8.3(4) |
| C13–Cg1–Cg2–C23 | 134.8(2) | O1–C1–C31–C32 | 30.7(4) |
| C14–Cg1–Cg2–C24 | 134.8(2) | O1–C1–C31–C36 | –143.8(3) |
| C15–Cg1–Cg2–C25 | 134.6(2) | O2–C2–C41–C42 | 145.1(3) |
| O1–C1–C11–C12 | 5.9(4) | O2–C2–C41–C46 | –31.5(4) |
| O1–C1–C11–C15 | –166.9(3) | | |

† Cg1 and Cg2 are the centroids of rings C11–C15 and C21–C25, respectively.

Table 2. Hydrogen-bonding geometry (\AA , $^\circ$) for (I)

| | | | | |
|-----------------------|---------------|-------------|-------------|-----------------------|
| $D\text{--}H\cdots A$ | $D\text{--}H$ | $H\cdots A$ | $D\cdots A$ | $D\text{--}H\cdots A$ |
| C14–H14...O2' | 0.93 | 2.55 | 3.354(4) | 145 |

Symmetry code: (i) $1 + x, y, z$.

Compound (II)

Crystal data

| | |
|---|---|
| [Fe(C ₅ H ₅)(C ₁₁ H ₈ NO ₂)] | Mo K α radiation |
| $M_r = 307.12$ | $\lambda = 0.7107 \text{ \AA}$ |
| Monoclinic | Cell parameters from 25 reflections |
| $P2_1/a$ | $\theta = 5.09\text{--}22.44^\circ$ |
| $a = 9.6988(11) \text{ \AA}$ | $\mu = 1.150 \text{ mm}^{-1}$ |
| $b = 9.3056(15) \text{ \AA}$ | $T = 294(1) \text{ K}$ |
| $c = 14.543(2) \text{ \AA}$ | Plate |
| $\beta = 93.311(12)^\circ$ | $0.33 \times 0.32 \times 0.04 \text{ mm}$ |
| $V = 1310.4(3) \text{ \AA}^3$ | Red |
| $Z = 4$ | |
| $D_x = 1.557 \text{ Mg m}^{-3}$ | |
| D_m not measured | |

Data collection

| | |
|-----------------------------------|--|
| Enraf–Nonius CAD-4 diffractometer | 1891 reflections with $I > 2\sigma(I)$ |
|-----------------------------------|--|

$\theta/2\theta$ scans
Absorption correction:
Gaussian
 $T_{\min} = 0.734$, $T_{\max} = 0.953$
3154 measured reflections
2990 independent reflections

$R_{\text{int}} = 0.024$
 $\theta_{\max} = 27.40^\circ$
 $h = -12 \rightarrow 12$
 $k = 0 \rightarrow 12$
 $l = 0 \rightarrow 18$
3 standard reflections
frequency: 120 min
intensity variation: 1%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.0403$
 $wR(F^2) = 0.1015$
 $S = 1.000$
2990 reflections
181 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.309 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.427 \text{ e } \text{\AA}^{-3}$
Extinction correction: none
Scattering factors from
International Tables for Crystallography (Vol. C)

Table 3. Selected geometric parameters (\AA , $^\circ$) for (II)

| | | | |
|-----------------|-----------|-----------------|------------|
| Fe1—Cg1† | 1.639 (2) | O2—N1 | 1.225 (4) |
| Fe1—Cg2 | 1.646 (2) | N1—C34 | 1.461 (4) |
| O1—N1 | 1.224 (4) | | |
| Cg1—Fe1—Cg2 | 179.3 (3) | O1—N1—C34 | 117.8 (3) |
| O1—N1—O2 | 124.2 (3) | O2—N1—C34 | 118.1 (3) |
| C11—Cg1—Cg2—C21 | 7.3 (3) | C12—C11—C31—C36 | -11.2 (4) |
| C12—Cg1—Cg2—C22 | 6.3 (3) | C15—C11—C31—C36 | 168.1 (3) |
| C13—Cg1—Cg2—C23 | 6.5 (3) | O1—N1—C34—C33 | 2.6 (4) |
| C14—Cg1—Cg2—C24 | 6.7 (3) | O2—N1—C34—C33 | -178.0 (3) |
| C15—Cg1—Cg2—C25 | 6.6 (3) | O1—N1—C34—C35 | -178.4 (3) |
| C12—C11—C31—C32 | 167.3 (3) | O2—N1—C34—C35 | 1.0 (4) |
| C15—C11—C31—C32 | -13.3 (4) | | |

† Cg1 and Cg2 are the centroids of rings C11–C15 and C21–C25, respectively.

Compounds (I) and (II) both crystallized in the monoclinic system, space groups $P2_1/n$ and $P2_1/a$, respectively, from the systematic absences. H atoms were treated as riding atoms with C—H 0.93 \AA .

For both compounds, data collection: *CAD-4-PC* (Enraf–Nonius, 1992); cell refinement: *SET4* and *CELDIM* in *CAD-4-PC*; data reduction: *DATRD2* in *NRCVAX96* (Gabe *et al.*, 1989); program(s) used to solve structures: *NRCVAX96* via Patterson heavy-atom method; program(s) used to refine structures: *NRCVAX96* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *NRCVAX96*, *ORTEPII* (Johnson, 1976), *PLATON* (Spek, 1997a) and *PLUTON* (Spek, 1997b); software used to prepare material for publication: *NRCVAX96*, *SHELXL97* and *WordPerfect* macro *PRPCIF97* (Ferguson, 1997).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1150). Services for accessing these data are described at the back of the journal.

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(1'-Benzoylferrocenyl)diphenylmethanol; a Centrosymmetric $R_4^4(16)$ Dimer Generated by C—H...O Hydrogen Bonding

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Abstract

In (1'-benzoylferrocenyl)diphenylmethanol, [(PhCO—C₅H₄)Fe(C₅H₄)]CPh₂OH (C₃₀H₂₄FeO₂), there is an intramolecular O—H...O hydrogen bond with O...O