

$\theta/2\theta$ 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 ($\text{\AA}$, $^\circ$) 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 $\text{\AA}$.

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).

JFG thanks the Research and Postgraduate Committee of Dublin City University, the Royal Irish Academy and Forbairt for generous funding of a research visit to the University of Guelph (June–August, 1997). SZA thanks the Committee of Vice-Chancellors and Principals (UK) and the University of St Andrews for financial support.

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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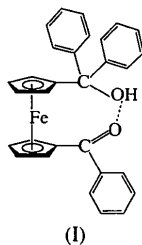
Abstract

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

2.891(2) Å; the ferrocenyl unit adopts an eclipsed conformation and the molecules are linked into centrosymmetric dimers by C—H···O hydrogen bonds with C···O 3.357(3) Å, to generate a cyclic $R_4^4(16)$ motif.

Comment

Substituted diphenylmethanols $R\text{CPh}_2\text{OH}$ exhibit a very wide range of hydrogen-bonding patterns in the solid state (Ferguson *et al.*, 1995). When R is ferrocenyl [(C₅H₅)Fe(C₅H₄)], the resulting ferrocenyl-diphenylmethanol, [(C₅H₅)Fe(C₅H₄)]CPh₂OH, crystallizes as cyclic centrosymmetric dimers (Ferguson *et al.*, 1993a) characterized by an (OH)₂ motif with graph set $R_2^2(4)$ (Bernstein *et al.*, 1995), while the analogous ferrocene-1,1'-diylbis(diphenylmethanol), Fe[(C₅H₄)CPh₂OH]₂, (in which both cyclopentadienyl rings carry a strong hydrogen-bond donor substituent) forms dimers based on an $R_4^4(8)$ motif in which the hydroxyl H atoms appear to be disordered (Ferguson *et al.*, 1993a), but are in fact mobile between pairs of non-equivalent sites (Aliev *et al.*, 1995). Continuing our study of the hydrogen-bonding patterns in ferrocenyl alcohols (Glidewell *et al.*, 1996), we have investigated the structure of (1'-benzoylferrocenyl)diphenylmethanol, [(PhCOC₅H₄)Fe(C₅H₄)]CPh₂OH, (I), in which the cyclopentadienyl ring not carrying the CPh₂OH substituent has a strong hydrogen-bond accepting benzoyl group. Compound (I) thus contains an excess of hard (Braga *et al.*, 1995) hydrogen-bond acceptors over hard donors, and consequently the occurrence of C—H···O hydrogen bonds is to be expected.



In compound (I) (Fig. 1), there are both intra- and intermolecular hydrogen bonds (Table 2). There is an intramolecular O—H···O hydrogen bond in which the hydroxyl and carbonyl O atoms act as a hydrogen-bond donor and acceptor, respectively, to give a motif whose graph set is $S(8)$; this resembles the intramolecular O—H···O hydrogen bond in Fe[(C₅H₄)CPh₂OH]₂ (Ferguson *et al.*, 1993a). In addition, there is an intermolecular C—H···O hydrogen bond; atom C53 in the benzoyl group (Fig. 1) at (x , y , z) acts as hydrogen-bond donor to the hydroxyl atom O1 at ($-x$, $2-y$, $-z$), while C53 at ($-x$, $2-y$, $-z$) in turn acts as a donor towards O1 at (x , y , z). In this way, a cyclic dimer is generated, with graph set $R_4^4(16)$ and lying about the inversion centre at (0,1,0) (Fig. 1). There are no short intermolecular

contacts involving the carbonyl O atom and it is noteworthy that it is the hydroxyl O atom which acts as the acceptor in the intermolecular C—H···O hydrogen bond, although the electrostatic nature of such interactions (Taylor & Kennard, 1982) means that carbonyl O atoms generally behave as more powerful hydrogen-bond acceptors than ether or alcohol O atoms (Desiraju, 1991, 1996).

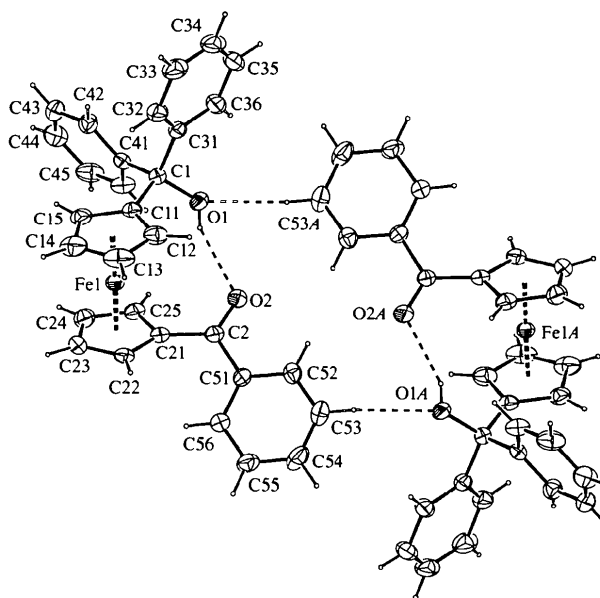


Fig. 1. A view of the dimeric aggregate in (I) showing the atom-numbering scheme, the O—H···O and C—H···O hydrogen bonds and the centrosymmetric $R_4^4(16)$ ring. Displacement ellipsoids are drawn at the 30% probability level.

Within the molecules of (I), the distances of the Fe atom from the centroid of the rings defined by C1 n and C2 n ($n = 1-5$) are 1.6437(4) and 1.6405(4) Å, respectively, and the angle subtended at the iron by the ring centroids is 176.65(2)°. There are three conformational variables of significance: the relative twist of the cyclopentadienyl rings and the conformation about the two independent exocyclic C—C bonds. A convenient measure of the relative twist of the rings is provided by the torsion angle C11—Cg1—Cg2—C21, where Cg1 and Cg2 represent the centroids of the two cyclopentadienyl rings; since the rings do not have local C₅ symmetry, the mean value of the torsion angles C1 n —Cg1—Cg2—C2 n (for $n = 1-5$) provides the appropriate measure; for perfect eclipsing of the rings, this value is (72 × n)°, where $n = 0$ or integer and $n = 0$ signifies that bonds C11—C1 and C21—C2 are also eclipsed. In compound (I), the mean twist angle is 70.4(1)°, indicative of nearly eclipsed rings with the exocyclic C—C bonds offset by one fifth of a revolution. This is the conformation in Fe[(C₅H₄)CPh₂OH]₂ (Ferguson *et al.*,

1993a) and in the majority of its adducts with hydrogen-bond acceptors (Ferguson *et al.*, 1993b; Glidewell *et al.*, 1994). The conformation about the exocyclic bonds C11—C1 and C21—C2 is defined by their torsion angles (Table 1); that for C11—C1 is very similar to the conformations observed in the simple ferrocenyl alcohol [(C₅H₅)Fe(C₅H₄)]CPh₂OH (Ferguson *et al.*, 1993a), as well as in the diol Fe[(C₅H₄)CPh₂OH]₂ and its adducts.

The bond lengths and angles show no unusual features: in particular, there is no significant difference between the mean C—C distances in the two differently substituted cyclopentadienyl rings. Examination of the structure with *PLATON* (Spek, 1997a) showed that there were no solvent-accessible voids in the crystal lattice.

Experimental

Compound (I) was prepared by reaction of 1,1'-dibenzoyl-ferrocene with phenyl magnesium bromide, followed by aqueous acidic workup. Purification was by chromatography on silica, with CH₂Cl₂ as eluent. Analysis: found C 75.5, H 5.3%; C₃₀H₂₄FeO₂ requires C 76.3, H 5.1%. NMR (CDCl₃ solution): δ_c 69.9 (*d*), 70.8 (*d*), 72.6 (*d*), 72.7 (*d*), 77.9 (*s*), 78.5 (*s*) (2 × C₅H₄); 99.3 (*s*, COH); 126.8(*d*), 126.9(*d*), 127.5(*d*), 128.3(*d*), 128.6(*d*), 132.2(*d*), 138.7(*s*), 147.3(*s*) (3 × C₆H₅), 200.3 (*s*, CO). Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation (at 273 K and in the dark) of an ethanol solution.

Crystal data

[Fe(C ₁₂ H ₉ O)(C ₁₈ H ₁₅ O)]	Mo K α radiation
$M_r = 472.34$	$\lambda = 0.7107 \text{ \AA}$
Monoclinic	Cell parameters from 25 reflections
$P2_1/n$	$\theta = 9.61\text{--}19.84^\circ$
$a = 13.3551(19) \text{ \AA}$	$\mu = 0.691 \text{ mm}^{-1}$
$b = 12.4868(8) \text{ \AA}$	$T = 294(1) \text{ K}$
$c = 14.7273(15) \text{ \AA}$	Plate
$\beta = 112.604(10)^\circ$	$0.35 \times 0.26 \times 0.08 \text{ mm}$
$V = 2267.3(4) \text{ \AA}^3$	Red
$Z = 4$	
$D_x = 1.384 \text{ Mg m}^{-3}$	
D_m not measured	

Data collection

Enraf–Nonius CAD-4 diffractometer	3298 reflections with $I > 2\sigma(I)$
ω – 2θ scans	$R_{\text{int}} = 0.012$
Absorption correction: Gaussian (ABSORB; Gabe <i>et al.</i> 1989)	$\theta_{\text{max}} = 29.0^\circ$
$T_{\text{min}} = 0.838$, $T_{\text{max}} = 0.944$	$h = -18 \rightarrow 16$
6533 measured reflections	$k = 0 \rightarrow 17$
6052 independent reflections	$l = 0 \rightarrow 20$
	3 standard reflections frequency: 240 min intensity variation: 1%

Refinement

Refinement on F^2	$(\Delta/\sigma)_{\text{max}} = 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$\Delta\rho_{\text{max}} = 0.237 \text{ e \AA}^{-3}$
$wR(F^2) = 0.097$	$\Delta\rho_{\text{min}} = -0.240 \text{ e \AA}^{-3}$

$S = 0.970$
6052 reflections
302 parameters
H atoms: see below
 $w = 1/[\sigma^2(F_o^2) + (0.0464P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

Extinction correction: none
Scattering factors from
International Tables for Crystallography (Vol. C)

Table 1. Selected geometric parameters ($\text{\AA}$, $^\circ$)

O1—C1	1.428 (2)	C12—C13	1.414 (4)
O2—C2	1.226 (2)	C13—C14	1.401 (4)
C1—C11	1.515 (3)	C14—C15	1.409 (3)
C1—C31	1.536 (3)	C21—C22	1.429 (3)
C1—C41	1.538 (3)	C21—C25	1.428 (3)
C2—C21	1.477 (3)	C22—C23	1.416 (3)
C2—C51	1.491 (3)	C23—C24	1.404 (3)
C11—C12	1.425 (3)	C24—C25	1.408 (3)
C11—C15	1.420 (3)		
O1—C1—C11	110.96 (16)	C31—C1—C41	109.61 (16)
O1—C1—C31	106.85 (17)	O2—C2—C21	119.71 (19)
C11—C1—C31	110.31 (18)	O2—C2—C51	119.50 (19)
O1—C1—C41	108.77 (17)	C21—C2—C51	120.66 (18)
C11—C1—C41	110.26 (17)		
O1—C1—C11—C15	−136.8 (2)	C11—C1—C31—C32	−24.0 (3)
C31—C1—C11—C15	105.0 (2)	O1—C1—C41—C42	−159.00 (19)
C41—C1—C11—C15	−16.2 (3)	C11—C1—C41—C42	79.1 (2)
O2—C2—C21—C25	32.2 (3)	O2—C2—C51—C52	9.9 (3)
O2—C2—C21—C22	−145.1 (2)	C21—C2—C51—C52	−174.30 (19)
O1—C1—C31—C32	−144.7 (2)		

Table 2. Hydrogen-bonding geometry ($\text{\AA}$, $^\circ$)

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
O1—H1 $\cdots$ O2	0.76 (2)	2.19 (3)	2.891 (2)	154 (3)
C53—H53 $\cdots$ O1 ⁱ	0.93	2.49	3.357 (3)	156

Symmetry code: (i) $-x, 2 - y, -z$.

Compound (I) crystallized in the monoclinic system; space group $P2_1/n$ from the systematic absences. H atoms attached to C atoms were allowed for as riding atoms with C—H 0.93 $\text{\AA}$; the hydroxy H atom was located from a difference map and refined isotropically.

Data collection: *CAD-4-PC* (Enraf–Nonius, 1992). Cell refinement: *SET4* and *CELDIM* in *CAD-4-PC*. Data reduction: *DATRED2* in *NRCVAX96* (Gabe *et al.*, 1989). Program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a). Program(s) used to refine structure: *NRCVAX96* and *SHELXL97* (Sheldrick, 1997b). 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).

GF thanks NSERC (Canada) for Research Grants, JFG thanks the Research and Postgraduate Committee of Dublin City University, the Royal Irish Academy and Forbairt for generous funding of a research visit to the University of Guelph (June–August, 1997). SZA thanks the Committee of Vice-Chancellors and Principals (UK) and the University of St Andrews for financial support.

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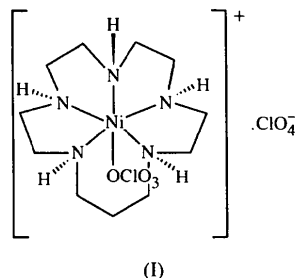
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one perchlorate O atom. There are two independent molecules in the asymmetric unit. The conformation of the ligand is in the most stable form, with the six-membered ring in a chair form and all four five-membered rings in *gauche* forms.

Comment

Polyaza macrocyclic ligands have attracted interest from coordination chemists, but most attention has been paid to tetradentate macrocycles, less information being available for larger ring systems. The Richman & Atkins (1974) procedure allows the simple and general synthesis of larger ring systems. Reported studies have been concerned with the thermodynamics and kinetics of the metal complexes of pentaaza macrocycles in solution (Kodama & Kimura, 1978*a,b*; Hay, Bembi, Moodie & Norman, 1982; Hay, Bembi, McLaren & Moodie, 1984). Little work has been carried out on the crystal structures of metal complexes of pentaaza macrocycles (Bombieri *et al.*, 1982; Eigenbrot *et al.*, 1988; Tahirov *et al.*, 1993). The present paper reports the crystal structure of the title compound, [Ni(ClO₄)(C₁₁N₅H₂₇)]ClO₄, (I).



The structure of (I) consists of two crystallographically independent [Ni(ClO₄)(C₁₁N₅H₂₇)]⁺ complex cations (denoted as molecules A and B) and two perchlorate anions. Both molecules have nearly the same conformation, and bond lengths and angles have normal values. The complex cation is six-coordinate, with five N atoms of the pentaaza macrocycle and a perchlorate O atom around the Ni^{II} ion. The macrocyclic ligand is coordinated with a 5,6,5 arrangement of the chelate rings in the equatorial plane containing four N atoms. The N3 and N4 atoms have opposite chirality giving the *meso-syn* diastereoisomer (Bombieri *et al.*, 1982). The configurations of the four chiral amine N centers are 1*RS*, 4*RS*, 10*SR* and 13*SR*. The conformation of the ligand is the most stable form, with the six-membered ring in a chair form and all four five-membered rings in *gauche* forms. The overall geometry is similar to that of an analogous cobalt(III) complex (Bombieri *et al.*, 1982). The crystal structure is stabilized by a three-dimensional network of N—H···O hydrogen bonds, as given in Table 2. The second perchlorate anion is free in the lattice and participates in the hydrogen bonding.

Acta Cryst. (1997). **C53**, 1778–1780

(1,4,7,11,13-Pentaazacyclohexadecane- κ^5 N)-(perchlorato- κ O)nickel(II) Perchlorate

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Abstract

The crystal structure of the title compound, [Ni(ClO₄)(C₁₁H₂₇N₅)]ClO₄, shows that the Ni^{II} ion is six-coordinate involving the pentadentate macrocycle and