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Ferrocenylbenzoic acid

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.055
wR factor = 0.150
Data-to-parameter ratio = 13.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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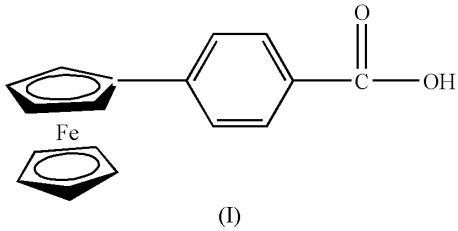
In the title compound, $[Fe(C_5H_5)(C_{12}H_9O_2)]$, there exists an extended conjugated system between the benzoic and cyclopentadienyl rings. The packing is stabilized by OH···O hydrogen bonds.

Comment

The study of ferrocene compounds opened up a new field of organometallic chemistry and has increased during the last two decades (Guo *et al.*, 2004). As non-benzenoid aromatic complexes, the physical and chemical properties of ferrocene compounds show unaccustomed variety due to the existence of the iron atom. They are used as combustion-improving agents for the solid propellant of hydroxyl-terminated polybutadiene binders, which contribute greatly to their fast development. In order to further explore this kind of complex, we report here the crystal structure of the title compound, (I).



(I)

In the title compound, the C—C bond lengths of the cyclopentadienyl rings are in good agreement with the values reported for other ferrocene derivatives (Wang *et al.*, 1970; Guo *et al.*, 2004). The Fe–C distances are also in good agreement with reported values (Dunitz *et al.*, 1956). The distances of the Fe atom from the centroids of the substituted and unsubstituted cyclopentadienyl rings [1.647 (2) and 1.642 (2) Å, respectively] are a little shorter than those found in ferrocene [1.660 (2) Å]. The C8—C11 bond distance [1.465 (8) Å] suggests partial double-bond character, indicating conjugation between the benzene and cyclopentadienyl rings. The dihedral angle between the C1–C5 and C6–C10 cyclopentadienyl rings of the ferrocene and the benzene ring are 5.61 (2) and 6.32 (2)°, respectively. There is an intermolecular OH···O hydrogen bond, which stabilizes the crystal structure (Table 1).

Experimental

The title compound was synthesized by reaction of *p*-aminobenzoic acid (0.07 mol), sodium nitrite (0.072 mol), HCl (140 ml, 4.3 *M*) and ferrocene (0.072 mol) at 273–278 K for 1 h. Single crystals suitable for

X-ray measurements were obtained by recrystallization from methanol at room temperature.

Crystal data

$[Fe(C_5H_5)(C_{12}H_9O_2)]$	D_x = 1.539 Mg m^{-3}
M_r = 306.13	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
a = 7.8880 (16) Å	θ = 4–14°
b = 16.006 (3) Å	μ = 1.14 mm^{-1}
c = 11.579 (4) Å	T = 293 (2) K
β = 115.38 (2)°	Pillar, red
V = 1320.8 (6) Å^3	0.20 × 0.20 × 0.18 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	θ_{max} = 26.0°
ω scans	$h = -9 \rightarrow 0$
Absorption correction: none	$k = -19 \rightarrow 0$
2768 measured reflections	$l = -12 \rightarrow 14$
2578 independent reflections	3 standard reflections
1192 reflections with $I > 2\sigma(I)$	every 100 reflections
R_{int} = 0.095	intensity decay: none

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.055	$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.150	$(\Delta/\sigma)_{max} < 0.001$
S = 0.96	$\Delta\rho_{max}$ = 0.49 e Å^{-3}
2578 reflections	$\Delta\rho_{min}$ = −0.43 e Å^{-3}
197 parameters	

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···O2^{i}	0.81 (6)	1.86 (6)	2.646 (6)	162 (7)

Symmetry code: (i) $-2-x, 1-y, -2-z$.

Carbon-bound H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2 times U_{eq}(C). The H atom attached to oxygen was located in a difference map and freely refined.

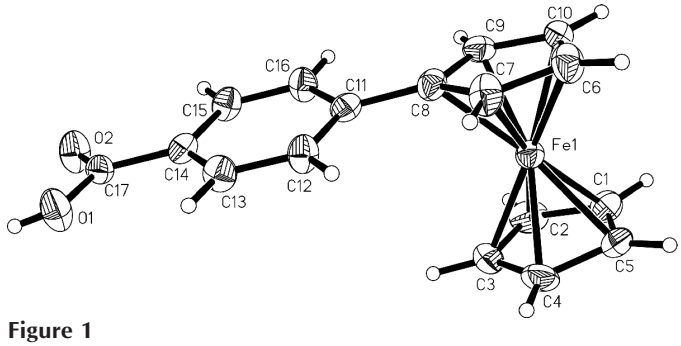


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXTL/PC* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL/PC*; software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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