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(4-Fluoro-3-nitrophenyl)ferrocene

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Key indicators

Single-crystal X-ray study
T = 446 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.100
Data-to-parameter ratio = 13.2

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

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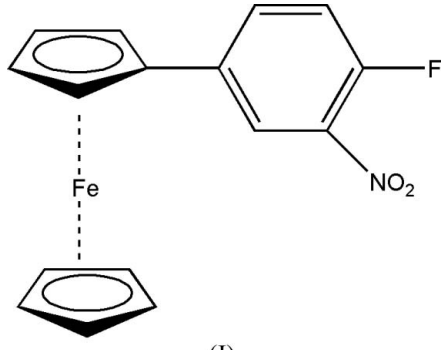
The title compound, $[Fe(C_5H_5)(C_{11}H_7FNO_2)]$, crystallizes with the 4-fluoro-3-nitrophenyl unit nearly coplanar with the cyclopentadienyl ring to which it is attached.

Comment

Compounds containing ferrocene building blocks have been widely studied owing to their potential uses in catalysis, materials science, molecular devices and hydrometallurgy (Hayashi *et al.*, 1989; Slone *et al.*, 1997). We report here the crystal structure of (I).



(I)

In (I) (Fig. 1), all bond lengths and angles are normal (Allen *et al.*, 1987; Gallagher *et al.*, 1997). The Fe···*Cg*1 and Fe···*Cg*2 distances are 1.651 (3) Å and 1.649 (2) Å, respectively, and the *Cg*1···Fe···*Cg*2 angle is 177.9 (3)°, where *Cg*1 and *Cg*2 are the centroids of the unsubstituted and substituted Cp rings, respectively. The 4-fluoro-3-nitrophenyl unit C11–C16/F1/N1/O1/O2 is coplanar with the cyclopentadienyl ring (C6—C10) to which it is attached, the largest deviation from the combined mean plane being 0.063 (2) Å for atom C7.

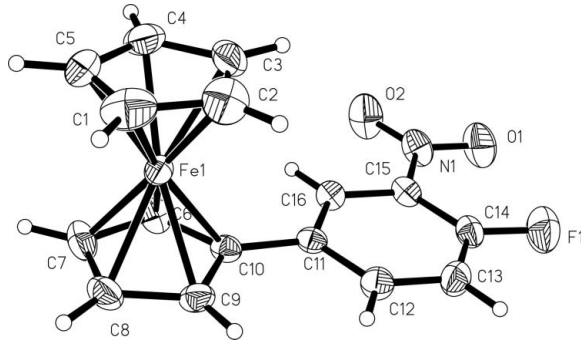


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

Although the nitro group is well established as a powerful acceptor of C—H···O hydrogen bonds (Sharma & Desiraju, 1994), there are no intermolecular contacts in (I) less than the sum of the van der Waals radii; in particular, there are no significant C—H···O interactions.

Experimental

The title compound was synthesized by the reaction of ferrocene (0.01 mol) with a freshly diazotized solution of 4-fluoro-3-nitroaniline (0.01 mol) in dilute sulfuric acid (15 ml), followed by chromatography on alumina, using dichloromethane–petroleum ether (1:1 *v*/*v*) as eluent. Crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of an ethyl acetate–dichloromethane (1:1 *v*/*v*) solution at room temperature over a period of one week.

Crystal data

$[Fe(C_5H_5)(C_{11}H_7FNO_2)]$
M_r = 325.12
Monoclinic, $P2_1/n$
a = 10.196 (2) Å
b = 12.905 (3) Å
c = 10.639 (2) Å
β = 104.882 (3)°
V = 1352.9 (5) Å^3
Z = 4
D_x = 1.596 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.13 mm^{-1}
T = 446 (2) K
Block, red
0.45 × 0.40 × 0.39 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.631, T_{max} = 0.667
6918 measured reflections
2510 independent reflections
2119 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.100
S = 1.05
2510 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2 + 0.3244P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.98 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1999); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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