Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

[(1-Phenylethyl)iminomethyl]ferrocene

Elmar Hecht‡

Universität Leipzig, Institut für Anorganische Chemie, Johannisallee 29, D-04103 Leipzig, Germany

‡ Present address: SusTech Darmstadt GmbH & Co KG, Petersenstraße 20, D-64287 Darmstadt, Germany

Correspondence e-mail:
elmar.hecht@sustech.de

Received 29 September 2004
Accepted 1 October 2004
Online 9 October 2004

The title Schiff base compound, $[Fe(C_5H_5)(C_{14}H_{14}N)]$, consists of discrete monomeric molecules separated by van der Waals contacts. The C═N bond length is 1.267 (3) Å. The ferrocenyl unit and the alkyl moiety bonded to the N atom of the imino group are arranged in *trans* positions.

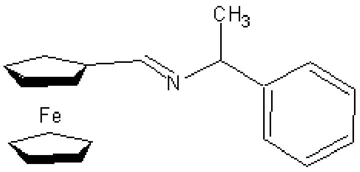
Key indicators

Single-crystal X-ray study
T = 213 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.084
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.

Comment

During the past decade optically active ferrocenyl compounds containing N-, O- and P-donor atoms have attracted considerable attention due to their possible application in the catalysis of enantioselective reactions (Richards & Locke, 1998; Togni, 2000). The structures of several Schiff base complexes containing a ferrocene unit have been reported (Carboni & Monnier, 1999; Enders *et al.*, 1997). The C═N bond distance [1.267 (3) Å] in the imino group of the title compound, (I), is generally consistent with those reported for other complexes of this type. The alkyl moiety in (I) occupies a *trans* position with respect to the ferrocenyl unit. The five membered rings of the ferrocene fragments are planar and parallel [dihedral angle = 3.2 (6)°].



(I)

Experimental

The title compound, (I), was prepared by reaction of 1-phenylethylamine (20 mmol) with ferrocenealdehyde (20 mmol) in tetrahydrofuran. The reaction mixture was refluxed for 2 h and the solvent removed *in vacuo* to give an orange precipitate. The solid was collected and dried *in vacuo*. Suitable crystals were obtained by cooling a saturated solution of (I) in diethyl ether. Analysis calculated for $C_{19}H_{19}FeN$: C 71.92, H 6.00, Fe 17.66%; found: C 72.11, H 6.23, Fe 17.38%.

Crystal data

$[Fe(C_5H_5)(C_{14}H_{14}N)]$
$M_r = 317.20$
Monoclinic, $P2_1$
$a = 5.9480$ (3) Å
$b = 7.5010$ (4) Å
$c = 17.3197$ (10) Å
$\beta = 92.751$ (1)°
$V = 771.84$ (7) Å^3
$Z = 2$
$D_x = 1.365$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3511 reflections
$\theta = 2$–25°
$\mu = 0.97$ mm^{-1}
$T = 213$ (2) K
Block, orange
0.40 × 0.30 × 0.20 mm

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Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.698$, $T_{\max} = 0.830$
5063 measured reflections
3511 independent reflections
3264 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\max} = 28.8°$
$h = -7 \rightarrow 6$
$k = -9 \rightarrow 10$
$l = -23 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.084$
$S = 1.12$
3511 reflections
266 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.0168P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.007$
$\Delta\rho_{\max} = 0.25$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}
Absolute structure: Flack (1983), 1416 Friedel pairs
Flack parameter = 0.011 (16)

Table 1
Selected geometric parameters (Å, °).

C14—C12	1.514 (3)	N1—C12	1.482 (3)
N1—C11	1.267 (3)	C12—C13	1.527 (4)
C11—N1—C12	115.5 (2)	N1—C12—C13	108.3 (2)
N1—C12—C14	110.7 (2)	C14—C12—C13	112.1 (2)

All H atoms were located in a difference Fourier map and freely refined.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97 and *PLATON* (Spek, 2003).

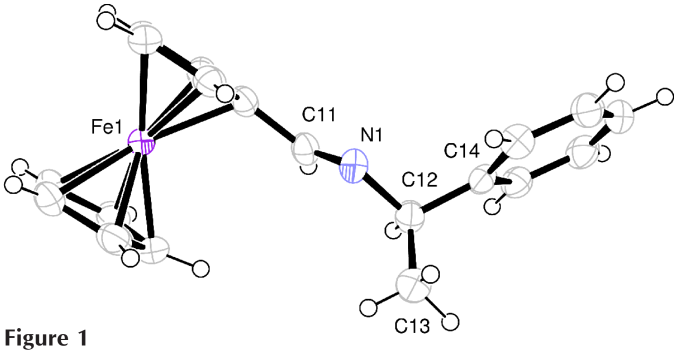

Figure 1
View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Financial support from the Deutsche Forschungsgemeinschaft is gratefully acknowledged.

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