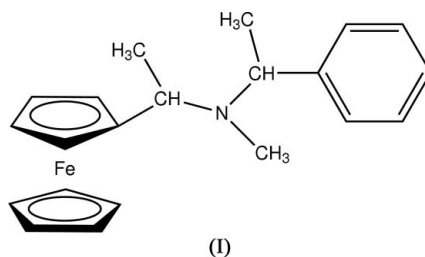


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## Key indicators

Single-crystal X-ray study  
 $T = 291$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.008$  Å  
 $R$  factor = 0.056  
 $wR$  factor = 0.130  
Data-to-parameter ratio = 15.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.***N*-(1-Ferrocenylethyl)-*N*-(1-phenylethyl)-  
methylamine**The title compound,  $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{16}\text{H}_{20}\text{N})]$ , was synthesized by reductive methylation of the corresponding secondary amine. In the crystal structure,  $\text{C}-\text{H}\cdots\pi$  interactions are observed between neighboring molecules.Received 4 January 2006  
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## Comment

Ferrocenylalkylamine derivatives have been used in asymmetric catalytic hydrogenation (Hayashi *et al.*, 1986), allylic substitution (Sawamura & Ito, 1992) and aldol reactions (Togni *et al.*, 1996). The structure of 1-ferrocenyl-*N*-(1-phenylethyl)ethylamine (Qian *et al.*, 2005) has been reported by our group. As part of our study of the cyclopalladation of tertiary amines, the crystal structure of the title compound, (I), is presented here.The molecular structure of (I) is shown in Fig.1, and selected bond lengths and angles are given in Table 1. The cyclopentadienyl rings of the ferrocene moiety are parallel to each other, with a dihedral angle of  $2.7(3)^\circ$ . Atom N1 is coplanar with the C11/C12/C13 plane, the deviation being  $0.022(4)$  Å. Atoms C11 and N1 are displaced from the benzene plane by  $1.308(5)$  and  $1.261(4)$  Å, respectively.In the crystal structure of (I), molecules are linked by  $\text{C}-\text{H}\cdots\pi$  interactions [ $\text{H}7\text{A}\cdots\text{Cg}1^{\text{i}} = 3.10$  Å and  $\text{C}7-\text{H}7\text{A}\cdots\text{Cg}1^{\text{i}} = 153^\circ$ , and  $\text{H}8\text{A}\cdots\text{Cg}2^{\text{ii}} = 3.14$  Å and  $\text{C}8-\text{H}8\text{A}\cdots\text{Cg}2^{\text{ii}} = 126^\circ$ , where  $\text{Cg}1$  and  $\text{Cg}2$  are the centroids of the C1-containing and C13-containing rings, respectively; symmetry codes: (i)  $1 - x, \frac{1}{2} + y, 1 - z$ ; (ii)  $1 - x, \frac{1}{2} + y, -z$ ].

## Experimental

Sodium borohydride (185 mg, 5 mmol) was added to a methanol solution (15 ml) containing  $\alpha$ -ferrocenyl-*N*-(1-phenylethyl)ethylamine (333 mg, 1 mmol) and 37% aqueous formaldehyde (1 ml, 12.5 mmol). The reaction mixture was stirred for 5 h at 273 K and evaporated under reduced pressure; the product was extracted with diethyl ether. The tertiary amine was purified by chromatography on silica gel developed with hexane–ethyl acetate (2:1) as eluant in 86% yield and recrystallized from dichloromethane/hexane (2:1). Single crystals of (I) were obtained after 3 d. IR (KBr,  $\nu$ ,  $\text{cm}^{-1}$ ): 3421, 3079,

2983, 1615, 1484, 1446, 1120, 1000, 822;  $^1\text{H NMR}$  ( $\text{CDCl}_3$ ):  $\delta$  7.25–7.39 (*m*, 5H), 4.10–4.11 (*m*, 4H), 4.02 (*s*, 5H), 3.79 (*d*  $\times$  *d*, 1H,  $J = 6.8$  Hz and  $J = 12.9$  Hz), 3.49 (*d*  $\times$  *d*, 1H,  $J = 6.4$  Hz and  $J = 12.6$  Hz), 1.92 (*s*, 3H) 1.37 (*d*, 3H,  $J = 6.8$  Hz), 1.24 (*d*, 3H,  $J = 6.4$  Hz); Elemental analysis calculated for  $\text{C}_{21}\text{H}_{25}\text{FeN}$ : C 72.62, H 7.20, N 4.03%; found: C 72.38, H 7.49, N 4.13%.

Crystal data

$[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{16}\text{H}_{20}\text{N})]$   
 $M_r = 347.27$   
 Monoclinic,  $P2_1$   
 $a = 5.8833$  (12) Å  
 $b = 10.748$  (2) Å  
 $c = 14.191$  (3) Å  
 $\beta = 97.82$  (3)°  
 $V = 889.0$  (3) Å<sup>3</sup>  
 $Z = 2$

$D_x = 1.297$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 714 reflections  
 $\theta = 2.1$ – $12.4$ °  
 $\mu = 0.85$  mm<sup>-1</sup>  
 $T = 291$  (2) K  
 Block, orange  
 $0.20 \times 0.18 \times 0.16$  mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Bruker, 2000)  
 $T_{\min} = 0.849$ ,  $T_{\max} = 0.876$   
 5026 measured reflections

3239 independent reflections  
 2928 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.060$   
 $\theta_{\text{max}} = 26.0$ °  
 $h = -7 \rightarrow 7$   
 $k = -13 \rightarrow 13$   
 $l = -17 \rightarrow 17$

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.056$   
 $wR(F^2) = 0.130$   
 $S = 1.07$   
 3239 reflections  
 208 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.55P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.33$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.45$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), 1394 Friedel Pairs  
 Flack parameter: 0.06 (3)

Table 1

Selected geometric parameters (Å, °).

N1–C12	1.489 (6)	C12–C13	1.517 (7)
N1–C11	1.497 (6)	C12–C21	1.532 (7)
C11–C19	1.522 (7)	C17–C18	1.390 (8)
C20–N1–C12	110.3 (4)	N1–C11–C10	107.4 (4)
C20–N1–C11	111.6 (4)	N1–C12–C13	110.1 (4)
C12–N1–C11	113.3 (4)	N1–C12–C21	111.3 (4)
N1–C11–C19	115.2 (4)		

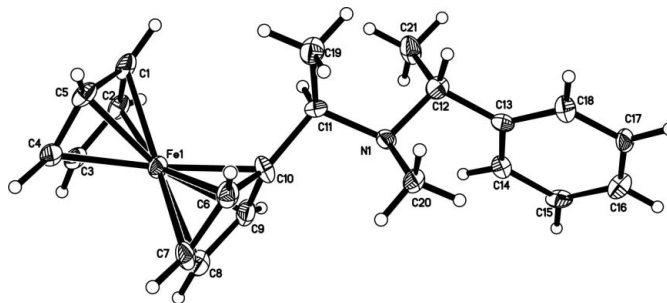


Figure 1

The structure of the molecule of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Methyl H atoms were placed in calculated positions, with C–H = 0.96 Å, and refined with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ . Other H atoms were placed in calculated positions, with C–H = 0.93–0.98 Å, and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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