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# 1-Ferrocenyl-1-(1-indenyl)cyclohexane

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**Key indicators**

Single-crystal X-ray study
$T$ = 294 K
Mean $\sigma$(C–C) = 0.005 Å
$R$ factor = 0.044
$wR$ factor = 0.121
Data-to-parameter ratio = 16.5

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



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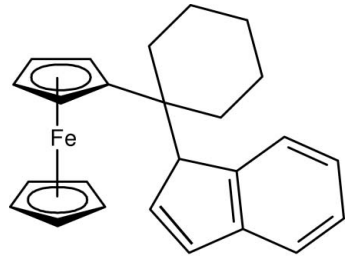
In the title compound, $[Fe(C_5H_5)(C_{20}H_{23})]$, the two five-membered cyclopentadienyl rings are nearly parallel, with a dihedral angle of only 3.8 (1)°. The dihedral angle between the indenyl plane and the substituted cyclopentadienyl ring is 58.1 (2)°.

## Comment

A number of ferrocene derivatives substituted with an indenyl group have been structurally characterized, including 2-ferrocenyl-2-(3-indenyl)propane (Gaede, 2000), 1-(ferrocenyl)indene and 2-(ferrocenyl)indene (Plenio, 1992). As a further contribution, we report here the synthesis and crystal structure of 1-ferrocenyl-1-(1-indenyl)cyclohexane, (I).




(I)

A view of (I) is shown in Fig. 1 and selected bond lengths and angles are listed in Table 1. The dihedral angle between the indenyl plane and the substituted cyclopentadienyl ring is 58.1 (2)°. The Fe atom is $\eta^5$-coordinated by both cyclopentadienyl rings, with distances ranging from 2.015 (4) (to C10) to 2.074 (3) Å (to C1). The two five-membered cyclopentadienyl rings are nearly parallel, forming a dihedral angle of only 3.8 (1)°. The cyclohexane ring has a normal chair conformation.

## Experimental

A solution of indene (1.39 ml, 12 mmol) in tetrahydrofuran (THF, 100 ml) was reacted with *n*-butyllithium (12 mmol) at 273 K for 2 h and then stirred at room temperature for 4 h. A solution of 6,6-pentamethylenefulvene (1.75 g, 12 mmol) in THF (20 ml) was added dropwise at 273 K with stirring. When the addition was complete, the solution was warmed to room temperature and stirring was continued overnight. Cyclopentadienyllithium (12 mmol) in THF (20 ml) was added to this reaction mixture, followed by $FeCl_2$·1.44THF (2.78 g, 12 mmol), and the mixture was then stirred overnight. The solvent was removed under vacuum. The residue was chromatographed through a short column of $Al_2O_3$ with $CH_2Cl_2$, yielding an orange solid, which was collected and purified by chromatography on alumina to give orange crystals (yield 1.24 g, 27.07%). Calculated for $C_{26}H_{28}Fe$: C 78.54, H 6.85%; found: C 78.65, H 6.61%.

*Crystal data*

| | |
|---|---|
| $[Fe(C_5H_5)(C_{20}H_{21})]$ | $D_x$ = 1.341 Mg m$^{-3}$ |
| $M_r$ = 382.31 | Mo $K\alpha$ radiation |
| Monoclinic, $P2_1/c$ | Cell parameters from 2652 reflections |
| $a$ = 13.232 (2) Å | $\theta$ = 2.3–24.3° |
| $b$ = 11.6546 (18) Å | $\mu$ = 0.80 mm$^{-1}$ |
| $c$ = 12.293 (2) Å | $T$ = 294 (2) K |
| $\beta$ = 92.881 (3)° | Block, orange |
| $V$ = 1893.4 (5) Å$^3$ | 0.26 × 0.24 × 0.18 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 3887 independent reflections |
| | 2407 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int}$ = 0.038 |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $\theta_{max}$ = 26.5° |
| | $h = -16 \rightarrow 16$ |
| $T_{min}$ = 0.793, $T_{max}$ = 0.866 | $k = -14 \rightarrow 6$ |
| 10458 measured reflections | $l = -15 \rightarrow 15$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.5012P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.044 | |
| $wR(F^2)$ = 0.121 | |
| $S$ = 1.01 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 3887 reflections | $\Delta\rho_{max}$ = 0.41 e Å$^{-3}$ |
| 235 parameters | $\Delta\rho_{min}$ = −0.30 e Å$^{-3}$ |
| H-atom parameters constrained | |

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Fe1—C1 | 2.074 (3) | Fe1—C6 | 2.021 (4) |
| Fe1—C2 | 2.046 (3) | Fe1—C7 | 2.035 (4) |
| Fe1—C3 | 2.028 (3) | Fe1—C8 | 2.024 (4) |
| Fe1—C4 | 2.023 (3) | Fe1—C9 | 2.026 (4) |
| Fe1—C5 | 2.037 (3) | Fe1—C10 | 2.015 (4) |

H atoms were placed in calculated positions, with C—H = 0.93–0.98 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: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

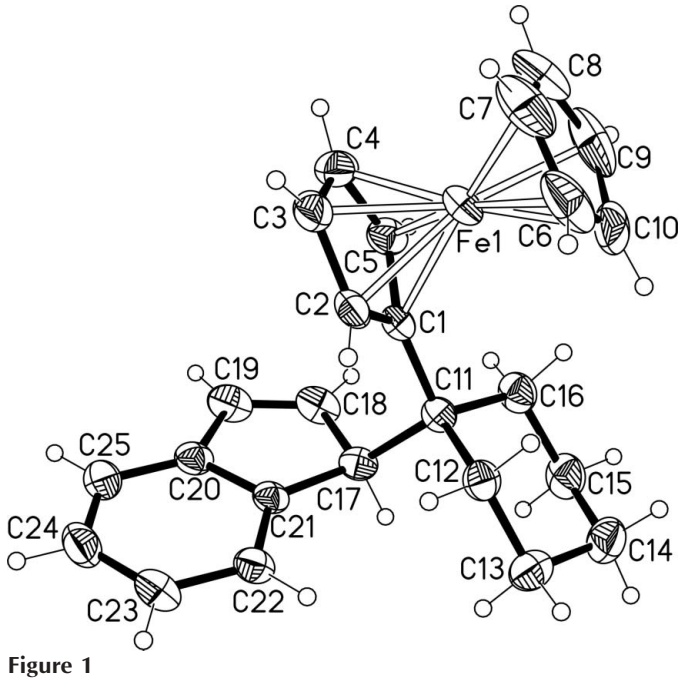



**Figure 1**
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

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