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(η^5-4,7-Dimethylindenyl)(η^5-pentamethylcyclopentadienyl)iron(II)

Peter G. Jones,[a]* Henning Hopf[b] and Thorsten Hartig[b]

[a]Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Postfach 3329, 38023 Braunschweig, Germany, and [b]Institut für Organische Chemie, Technische Universität Braunschweig, Postfach 3329, 38023 Braunschweig, Germany

Correspondence e-mail:
jones@xray36.anchem.nat.tu-bs.de

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Key indicators

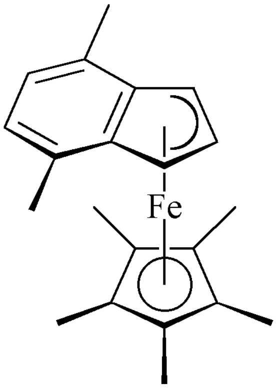
Single-crystal X-ray study
T = 178 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.089
Data-to-parameter ratio = 13.4

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

The molecule of the title compound, [Fe($C_{10}H_{15}$)($C_{11}H_{11}$)], contains parallel and eclipsed five-membered rings coordinated to the central Fe atom at perpendicular distances of 1.642 (1) (cyclopentadienyl ring) and 1.667 (1) Å (indenyl ring).

Comment

In our studies of the preparation and uses of novel metallocenes containing the [2.2]paracyclophane unit (Hopf *et al.*, 2002), we needed the title ferrocene, (I), which incorporates a 'half-cyclophane' as a subunit, as a reference compound. Here, we present its structure.



(I)

The molecule is shown in Fig. 1. The five-membered rings are planar (mean deviation 0.008 Å for C1 to C7*A* and 0.002 Å for C15 to C19), essentially parallel [interplanar angle 2.8 (2)°] and almost ideally eclipsed [torsion angle *e.g.* C2—Cent1—Cent2—C16 −0.3 (2)°, where Cent represents the centroid of the ring C atoms]. The perpendicular distance of the Fe atom from the rings is 1.667 (1) and 1.642 (1) Å, respectively. The coordination to the indenyl ring is very slightly distorted towards η^3, the distances Fe—C3*A* and Fe—C7*A* being significantly longer than the others (Table 1).

The molecules pack (Fig. 2) in layers parallel to the *ab* plane, with a herring-bone pattern.

Experimental

The title compound was prepared in 85% yield (Hartig, 1991) by first metallating 4,7-dimethyl-1*H*-indene with methyl lithium in anhydrous tetrahydrofuran and then quenching the anion thus formed with an equivalent amount of the complex [(C_5Me_5)Fe(CH_3CN)$_3$]PF_6. Crystals were grown by cooling of a hot saturated solution in hexane.

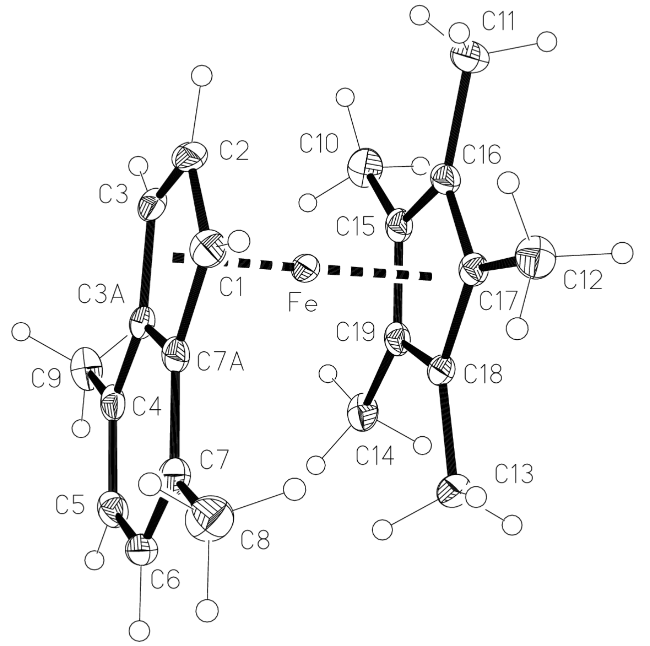


Figure 1
The molecule of the title compound in the crystal. Ellipsoids are drawn at the 30% probability level.

Crystal data

$[Fe(C_{10}H_{15})(C_{11}H_{11})]$
$M_r = 334.27$
Monoclinic, $P2_1/n$
$a = 8.350\ (2)$ Å
$b = 13.925\ (3)$ Å
$c = 14.645\ (4)$ Å
$\beta = 95.88\ (2)^\circ$
$V = 1693.9\ (7)$ Å^3
$Z = 4$

$D_x = 1.311$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 48 reflections
$\theta = 10–12^\circ$
$\mu = 0.89$ mm^{-1}
$T = 178\ (2)$ K
Tablet, red
$0.60 \times 0.40 \times 0.15$ mm

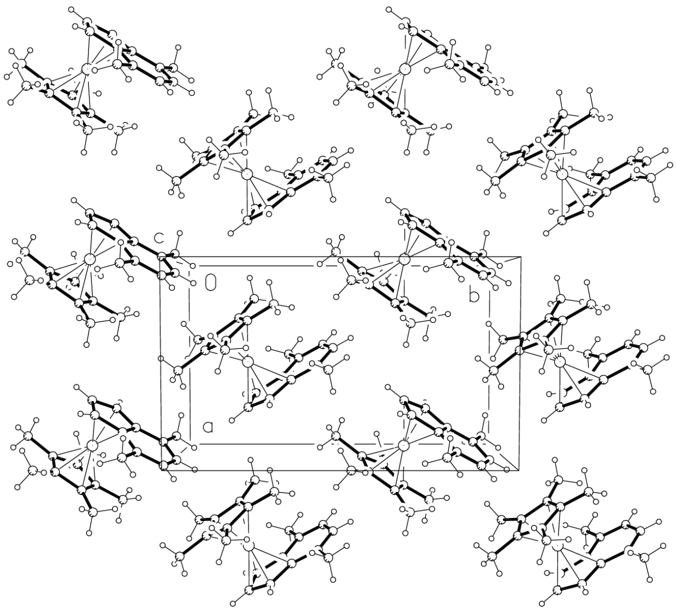


Figure 2
Packing diagram of the title compound with view direction parallel to the *c* axis. There are two such layers, related by inversion symmetry, per *c* axis repeat. Radii are arbitrary.

Data collection

Nicolet *R*3 diffractometer
ω scans
Absorption correction: none
2821 measured reflections
2768 independent reflections
2191 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$

$\theta_{\rm max} = 25.0^\circ$
$h = -9 \rightarrow 9$
$k = -16 \rightarrow 0$
$l = -17 \rightarrow 17$
3 standard reflections
every 247 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.089$
$S = 1.04$
2768 reflections
206 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.6303P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.37$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.46$ e Å^{-3}

Table 1
Selected interatomic distances (Å).

Fe—C16	2.037 (3)	C3—C3*A*	1.434 (4)
Fe—C2	2.039 (2)	C3*A*—C4	1.429 (4)
Fe—C15	2.040 (3)	C3*A*—C7*A*	1.440 (4)
Fe—C17	2.044 (3)	C4—C5	1.356 (4)
Fe—C3	2.045 (3)	C5—C6	1.427 (4)
Fe—C18	2.046 (2)	C6—C7	1.360 (4)
Fe—C19	2.049 (2)	C7—C7*A*	1.431 (4)
Fe—C1	2.049 (3)	C15—C19	1.432 (4)
Fe—C3*A*	2.089 (3)	C15—C16	1.433 (4)
Fe—C7*A*	2.093 (3)	C16—C17	1.432 (4)
C1—C2	1.414 (4)	C17—C18	1.425 (3)
C1—C7*A*	1.427 (4)	C18—C19	1.425 (4)
C2—C3	1.423 (4)		

H atoms at sp^2 C atoms were included using a riding model, starting from idealized positions. Methyl H atoms were located in difference syntheses, idealized and refined as rigid groups allowed to rotate but not tip.

Data collection: *P*3 (Nicolet, 1987); cell refinement: *P*3; data reduction: *XDISK* (Nicolet, 1987); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

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