Crystal structure of 1,1'-dibenzylferrocene, $C_{24}H_{22}Fe$

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$C_{24}H_{22}Fe$, monoclinic, $P12_1/a1$ (No. 14),
 $a = 15.804(9) \text{ \AA}$, $b = 6.034(4) \text{ \AA}$, $c = 9.437(6) \text{ \AA}$,
 $\beta = 97.79(1)^\circ$, $V = 891.6 \text{ \AA}^3$, $Z = 2$, $R(F) = 0.054$,
 $R_w(F) = 0.064$.

Source of material: The reduction of 1,1'-dibenzoylferrocene by dimethylsulfide-borane in THF with the CBS catalyst was previously described (see ref. 1) to yield the corresponding diol in high enantiomeric excess. On replacement of THF by toluene, the overreduction of the ketone functions has resulted in the title compound.

The Fe atom of the molecular unit, located on an inversion center, is surrounded by a centrosymmetric neighborhood of ten C atoms at distances ranging from 2.025(7) Å to 2.048(7) Å.

Table 1. Parameters used for the X-ray data collection

Crystal:	yellow plate, size 0.10 x 0.35 x 0.56 mm
Wavelength:	Mo $K\alpha$ radiation (0.7107 Å)
μ :	8.71 cm ⁻¹
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	ω
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	40°
$N(hkl)_{\text{unique}}$:	652
Criterion for I_o :	$I_o > 3 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	160
Programs:	SAPI91, teXsan

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{iso}
H(1)	4e	0.129(4)	0.78(1)	0.044(7)	0.04(2)
H(2)	4e	-0.028(6)	0.90(2)	0.11(1)	0.12(4)
H(3)	4e	-0.075(5)	0.56(1)	0.245(7)	0.06(2)
H(4)	4e	0.034(5)	0.26(2)	0.239(8)	0.08(3)
H(6')	4e	0.176(4)	0.20(1)	0.075(6)	0.04(2)
H(6'')	4e	0.196(4)	0.44(1)	0.022(6)	0.03(2)
H(8)	4e	0.228(4)	0.02(1)	0.290(6)	0.03(2)
H(9)	4e	0.317(5)	-0.02(2)	0.495(8)	0.07(3)
H(10)	4e	0.421(4)	0.25(1)	0.542(6)	0.04(2)
H(11)	4e	0.418(6)	0.60(2)	0.411(9)	0.11(3)
H(12)	4e	0.314(4)	0.61(1)	0.213(7)	0.05(2)

References

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Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe	2c	0	1/2	0	0.0269(8)	0.0324(9)	0.0315(8)	-0.0030(8)	0.0015(6)	-0.0058(8)
C(1)	4e	0.0952(5)	0.700(1)	0.0909(7)	0.035(4)	0.047(5)	0.030(4)	-0.006(4)	-0.003(3)	-0.001(4)
C(2)	4e	0.0170(5)	0.761(1)	0.1383(8)	0.047(5)	0.046(5)	0.045(4)	0.000(5)	-0.006(4)	-0.015(4)
C(3)	4e	-0.0123(5)	0.574(1)	0.2078(7)	0.042(5)	0.072(7)	0.030(4)	0.002(5)	0.001(4)	-0.021(4)
C(4)	4e	0.0484(5)	0.402(1)	0.2025(8)	0.045(5)	0.036(5)	0.039(4)	-0.005(4)	0.005(4)	0.001(4)
C(5)	4e	0.1139(4)	0.478(1)	0.1304(7)	0.039(4)	0.035(5)	0.032(4)	-0.008(4)	-0.004(3)	-0.005(4)
C(6)	4e	0.1908(5)	0.348(2)	0.1005(9)	0.037(5)	0.040(6)	0.059(5)	0.017(4)	0.000(4)	-0.003(5)
C(7)	4e	0.2577(4)	0.323(1)	0.2297(7)	0.024(4)	0.052(6)	0.029(4)	0.001(4)	0.006(3)	-0.002(4)
C(8)	4e	0.2582(5)	0.136(2)	0.3160(9)	0.051(5)	0.040(6)	0.061(5)	0.004(5)	0.012(4)	0.000(5)
C(9)	4e	0.3172(6)	0.111(2)	0.4351(9)	0.058(6)	0.060(6)	0.053(5)	0.016(5)	0.009(4)	0.024(5)
C(10)	4e	0.3759(5)	0.275(2)	0.4718(8)	0.030(4)	0.093(7)	0.041(5)	0.013(5)	-0.014(4)	0.012(5)
C(11)	4e	0.3747(5)	0.463(2)	0.3893(9)	0.050(5)	0.070(7)	0.053(5)	-0.009(5)	-0.003(4)	0.003(5)
C(12)	4e	0.3157(5)	0.482(2)	0.2705(8)	0.030(4)	0.057(6)	0.050(5)	0.002(5)	-0.007(4)	0.009(5)