Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(4-Bromophenyl)ferrocene

Vincent O. Nyamori and Muhammad D. Bala*

School of Chemistry, University of KwaZulu-Natal, Westville Campus, Private Bag X54001, Durban 4000, South Africa
Correspondence e-mail: bala@ukzn.ac.za

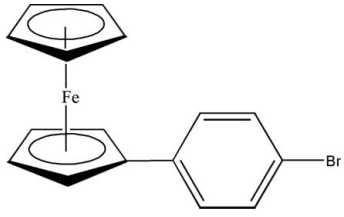
Received 25 August 2008; accepted 1 October 2008

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.030; wR factor = 0.075; data-to-parameter ratio = 19.2.

In the title compound, $[Fe(C_5H_5)(C_{11}H_8Br)]$, the distance of the Fe atom from the centroids of the unsubstituted and substituted cyclopentadienyl (Cp) rings is 1.644 (1) and 1.643 (1) Å, respectively. The ferrocenyl moiety deviates from an eclipsed geometry, with marginally tilted Cp rings and an interplanar angle between the Cp and benzene rings of 13.0 (4)°. The crystal structure is stabilized by C—H$\cdots\pi$ interactions between a cyclopentadienyl H atom and the cyclopentadienyl ring of a neighbouring molecule.

Related literature

For related literature, see: Allen (2002); Anderson *et al.* (2003); Cambridge Crystallographic Data Centre (2002); Coe *et al.* (1994); Hor *et al.* (1991); Imrie *et al.* (2002, 2003); Knoesen & Lotz (1999); Togni & Hayashi (1995).



Experimental

Crystal data

$[Fe(C_5H_5)(C_{11}H_8Br)]$
M_r = 341.02
Monoclinic, $P2_1/c$
a = 16.4991 (3) Å
b = 9.9578 (2) Å
c = 7.9269 (1) Å
β = 97.084 (1)°
V = 1292.41 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.24 mm^{-1}
T = 173 (2) K
0.37 × 0.32 × 0.07 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: integration (*XPREP*; Bruker, 2005)
T_{min} = 0.303, T_{max} = 0.756
15480 measured reflections
3126 independent reflections
2775 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.075
S = 1.15
3126 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C1–C5 cyclopentadienyl ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$\cdots Cg1^{i}$	0.95	2.90	3.780 (4)	154

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2005); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2003) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL*.

The authors thank Dr Manuel Fernandez for data collection, and the University of KwaZulu-Natal and the NRF for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2069).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Anderson, F. P., Gallagher, J. F., Kenny, P. T. M., Ryan, C. & Savage, D. (2003). *Acta Cryst.* C**59**, m13–m15.
Bruker (2005). *APEX2* and *SAINT-Plus* (includes *XPREP*). Bruker AXS Inc., Madison, Wisconsin, USA.
Cambridge Crystallographic Data Centre (2002). *CONQUEST*. Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ.
Coe, B. J., Foulon, J.-D., Hamor, T. A., Jones, C. J., McCleverty, J. A., Bloor, D., Cross, G. H. & Axon, T. L. (1994). *J. Chem. Soc. Dalton Trans.* pp. 3427–3439.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hor, T. S. A., Chan, H. S. O., Tan, K.-L., Phang, L.-T., Yan, Y. K., Liu, L. K. & Wen, Y.-S. (1991). *Polyhedron*, pp. 2437–2441.
Imrie, C., Engelbrecht, P., Loubser, C., McCleland, C. W., Nyamori, V. O., Bogadi, R., Levendis, D. C., Tolom, N., Rooyen, J. & Williams, N. (2002). *J. Organomet. Chem.* **645**, 65–81.
Imrie, C., Loubser, C., Engelbrecht, P., McCleland, C. W. & Zheng, Y. (2003). *J. Organomet. Chem.* **665**, 48–64.
Knoesen, O. & Lotz, S. (1999). *Technetium, Rhenium and other Metals in Chemistry and Nuclear Medicine*, edited by M. Nicolini & C. I. Mazzi, pp. 153–156. Padova: S. G. Editoriali.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Togni, A. & Hayashi, T. (1995). *Ferrocenes.* Weinheim: VCH.

supplementary materials

Acta Cryst. (2008). E**64**, m1376 [**doi:10.1107/S1600536808031759**]

1-(4-Bromophenyl)ferrocene

V. O. Nyamori and M. D. Bala

Comment

Ferrocene compounds especially those synthesized by reacting a *para*-substituted phenylferrocene 4-Fc—C_6H_4-*R* (*R* = any atom or group) are of great interest in the field of material chemistry (Togni & Hayashi, 1995). They are employed as precursors in the synthesis of ferrocenomesogens with the ferrocenyl moiety incorporated as a terminal group (Imrie *et al.*, 2002, 2003). Interest in these compounds stems from their potential use either as metathesis catalysts or therapeutic radiopharmaceuticals (Hor *et al.*, 1991; Knoesen & Lotz, 1999). The compounds have also been used to synthesize non-linear optical materials containing molybdenum or tungsten redox centres (Coe *et al.*,1994).

In the title compound (I, Fig. 1), the distance of the Fe atom from the centroids of the unsubstituted (C1—C5) and the substituted (C6—C10) cyclopentadienyl rings are 1.644 (1) and 1.643 (1) Å respectively, indicating that the *para*- substitution (bromophenyl group) has little influence on Fe—Cp bonding interactions. The two Cp rings deviate from an eclipsed conformation with torsion angles around 11.0 (2)°. The rings are also marginally tilted towards each other with a tilt angle between the planes of the two rings of 0.83 (2)°. The interplanar angle between the Cp and the phenyl rings of (I) was 13.0 (4)°. This value is very close to the 12.8° observed by Anderson *et al.* (2003) as the median value upon analysis of 17 structures from the April 2002 version of the Cambridge Structural Database using *ConQuest* Version 1.4 (Allen, 2002). The molecular packing (Fig. 2) is stabilized by C—H···π interactions between a cyclopentadienyl H atom and the cyclopentadienyl ring of an adjacent molecule, with a C2—H2···Cg^{i} separation of 2.90 Å (Fig. 2 and Table 1; Cg is the centroid of the C1-C5 cyclopentadienyl ring, symmetry code as in Fig. 2).

Experimental

The title compound (I) was synthesized *via* the diazonium reaction as follows: A solution of 4-bromobenzene diazonium sulfate was prepared by the reaction of 4-bromoaniline (20.02 g, 0.12 mol) in dilute sulfuric acid (100 cm^3) to which sodium nitrite (11.65 g, 0.17 mol) was slowly added in water at 278 K. The reaction temperature was continually monitored and held at 278 K during the addition. The resultant solution was filtered and the filtrate was immediately added to a cold, well stirred solution of ferrocene(24.60 g, 0.13 mol) in diethyl ether (450 cm^3). Stirring was continued at 278 K for 3 h and then at room temperature for a further 12 h. The ether layer was separated, washed with water, dried over anhydrous sodium sulfate and evaporated. The residue was purified by column chromatography on silica gel. Hexane was used to elute unreacted ferrocene and the product was eluted from the column using 1 : 1 hexane : dichloromethane mixture to yield 4.57 g, 11% of pure (I). mp 122–123 °C; Spectroscopic analysis: IR ν_{max}(KBr/cm^{-1}) 3086, 3053, 2925, 2853, 1588, 1509, 1446, 1406, 1383, 1278, 1103, 1088, 1066,1050, 1030, 1001, 884, 819; ^{1}H NMR ($CDCl_3$, 300 MHz) δ_H 7.41 (2*H*, d, *J* 8.5, ArH), 7.34 (2*H*, d, *J* 8.5, ArH), 4.62 (2*H*, t, *J* 1.8, C_5H_4),4.34 (2*H*, t, *J* 1.8, C_5H_4), 4.04 (5*H*, s, C_5H_5);

EI–MS 70 eV *m/z* 343 (18), 342 (96), 341 (22), 340 (M^+, 100), 260 (3), 205 (23), 203 (10), 202 (9); Elemental analysis (Found: C, 56.4; H, 3.8%; *M*, 339.9551. required for $C_{16}H_{13}FeBr$: C, 56.6; H, 3.9%; *M*, 339.9550).

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

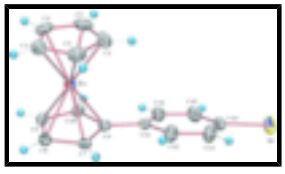


Fig. 1. Molecular structure of the title complex with the atom labelling scheme. Ellipsoids are drawn at the 50% probability level.

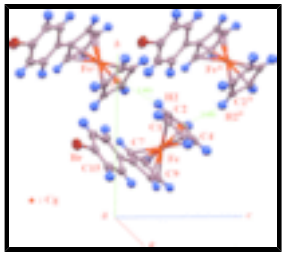


Fig. 2. A stereoview of the interactions in the crystal structure of (I). [Symmetry code: (i) x, -y+3/2, z-1/2; (ii) x, -y+3/2, z+1/2.]

1-(4-Bromophenyl)ferrocene

Crystal data

$[Fe(C_5H_5)(C_{11}H_8Br)]$	F_{000} = 680
M_r = 341.02	D_x = 1.753 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point = 395–396 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 16.4991 (3) Å	Cell parameters from 8414 reflections
b = 9.9578 (2) Å	θ = 2.4–28.4°
c = 7.9269 (1) Å	μ = 4.24 mm^{-1}
β = 97.084 (1)°	T = 173 (2) K
V = 1292.41 (4) Å^3	Plate, orange
Z = 4	0.37 × 0.32 × 0.07 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	3126 independent reflections
Radiation source: fine-focus sealed tube	2775 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
Detector resolution: 10.0 pixels mm^{-1}	θ_{max} = 28.0°
T = 173(2) K	θ_{min} = 1.2°
φ and ω scans	h = −21→21
Absorption correction: integration (XPREP; Bruker, 2005)	k = −13→13

T_{min} = 0.303, T_{max} = 0.756
15480 measured reflections

l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.075
S = 1.15
3126 reflections
163 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0124P)^2 + 2.8125P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br	−0.055964 (19)	0.43903 (4)	−0.29425 (5)	0.04324 (11)
Fe	0.35189 (2)	0.48664 (4)	0.27601 (5)	0.01850 (9)
C1	0.27574 (19)	0.6354 (3)	0.3370 (4)	0.0346 (7)
H1	0.2256	0.6612	0.2732	0.042*
C2	0.3538 (2)	0.6885 (3)	0.3185 (4)	0.0307 (7)
H2	0.3653	0.7560	0.2401	0.037*
C3	0.41137 (19)	0.6237 (3)	0.4365 (4)	0.0308 (6)
H3	0.4686	0.6397	0.4520	0.037*
C4	0.3689 (2)	0.5298 (3)	0.5287 (4)	0.0334 (7)
H4	0.3925	0.4720	0.6167	0.040*
C5	0.2854 (2)	0.5381 (3)	0.4659 (4)	0.0360 (7)
H5	0.2428	0.4865	0.5043	0.043*
C6	0.29438 (16)	0.3883 (3)	0.0676 (3)	0.0208 (5)
C7	0.36479 (16)	0.4587 (3)	0.0264 (3)	0.0225 (5)
H7	0.3652	0.5272	−0.0568	0.027*
C8	0.43450 (17)	0.4078 (3)	0.1324 (4)	0.0261 (6)

H8	0.4894	0.4363	0.1313	0.031*
C9	0.40733 (18)	0.3072 (3)	0.2393 (4)	0.0258 (6)
H9	0.4408	0.2569	0.3226	0.031*
C10	0.32169 (18)	0.2951 (3)	0.2001 (4)	0.0237 (6)
H10	0.2879	0.2350	0.2529	0.028*
C11	0.20996 (16)	0.4044 (3)	−0.0135 (3)	0.0213 (5)
C12	0.18754 (19)	0.5119 (3)	−0.1218 (4)	0.0309 (6)
H12	0.2269	0.5785	−0.1392	0.037*
C13	0.1081 (2)	0.5237 (3)	−0.2055 (4)	0.0340 (7)
H13	0.0933	0.5970	−0.2797	0.041*
C14	0.05166 (17)	0.4264 (3)	−0.1775 (4)	0.0295 (6)
C15	0.07133 (19)	0.3200 (3)	−0.0704 (4)	0.0337 (7)
H15	0.0314	0.2545	−0.0526	0.040*
C16	0.15020 (18)	0.3097 (3)	0.0114 (4)	0.0285 (6)
H16	0.1640	0.2364	0.0862	0.034*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.02264 (15)	0.0582 (2)	0.0466 (2)	0.00362 (14)	−0.00493 (13)	−0.00758 (17)
Fe	0.02091 (18)	0.01753 (18)	0.01723 (19)	−0.00139 (14)	0.00303 (14)	−0.00126 (14)
C1	0.0301 (15)	0.0309 (16)	0.0423 (19)	0.0082 (13)	0.0019 (13)	−0.0127 (14)
C2	0.0456 (18)	0.0172 (13)	0.0304 (16)	−0.0021 (12)	0.0082 (14)	−0.0022 (11)
C3	0.0297 (15)	0.0293 (15)	0.0330 (16)	−0.0040 (12)	0.0022 (12)	−0.0130 (12)
C4	0.054 (2)	0.0295 (15)	0.0171 (14)	0.0031 (14)	0.0049 (13)	−0.0048 (11)
C5	0.0425 (18)	0.0341 (17)	0.0358 (18)	−0.0090 (14)	0.0226 (14)	−0.0120 (14)
C6	0.0250 (13)	0.0199 (12)	0.0178 (13)	−0.0013 (10)	0.0036 (10)	−0.0017 (10)
C7	0.0237 (13)	0.0271 (14)	0.0174 (13)	−0.0009 (11)	0.0057 (10)	−0.0008 (10)
C8	0.0214 (13)	0.0325 (15)	0.0243 (14)	0.0014 (11)	0.0026 (11)	−0.0061 (11)
C9	0.0294 (14)	0.0239 (13)	0.0231 (14)	0.0055 (11)	−0.0015 (11)	−0.0036 (11)
C10	0.0313 (14)	0.0180 (12)	0.0217 (14)	−0.0025 (11)	0.0023 (11)	−0.0018 (10)
C11	0.0231 (13)	0.0225 (13)	0.0187 (13)	−0.0003 (10)	0.0037 (10)	−0.0032 (10)
C12	0.0292 (15)	0.0301 (15)	0.0325 (16)	−0.0060 (12)	−0.0003 (12)	0.0061 (12)
C13	0.0328 (16)	0.0331 (16)	0.0337 (17)	0.0012 (13)	−0.0051 (13)	0.0047 (13)
C14	0.0180 (12)	0.0402 (17)	0.0296 (16)	0.0027 (12)	0.0007 (11)	−0.0085 (13)
C15	0.0250 (14)	0.0360 (16)	0.0406 (18)	−0.0068 (13)	0.0061 (13)	−0.0038 (14)
C16	0.0275 (14)	0.0272 (14)	0.0307 (16)	−0.0028 (11)	0.0038 (12)	0.0026 (12)

Geometric parameters (Å, °)

Br—C14	1.902 (3)	C6—C7	1.429 (4)
Fe—C3	2.033 (3)	C6—C10	1.432 (4)
Fe—C4	2.034 (3)	C6—C11	1.469 (4)
Fe—C5	2.035 (3)	C7—C8	1.431 (4)
Fe—C7	2.035 (3)	C7—H7	0.9500
Fe—C2	2.037 (3)	C8—C9	1.420 (4)
Fe—C8	2.038 (3)	C8—H8	0.9500
Fe—C1	2.039 (3)	C9—C10	1.414 (4)
Fe—C10	2.043 (3)	C9—H9	0.9500

Fe—C9	2.044 (3)	C10—H10	0.9500
Fe—C6	2.050 (3)	C11—C12	1.394 (4)
C1—C5	1.403 (5)	C11—C16	1.396 (4)
C1—C2	1.417 (4)	C12—C13	1.399 (4)
C1—H1	0.9500	C12—H12	0.9500
C2—C3	1.405 (4)	C13—C14	1.381 (4)
C2—H2	0.9500	C13—H13	0.9500
C3—C4	1.424 (5)	C14—C15	1.371 (5)
C3—H3	0.9500	C15—C16	1.384 (4)
C4—C5	1.408 (5)	C15—H15	0.9500
C4—H4	0.9500	C16—H16	0.9500
C5—H5	0.9500		
C3—Fe—C4	40.98 (13)	Fe—C3—H3	126.1
C3—Fe—C5	68.36 (13)	C5—C4—C3	107.6 (3)
C4—Fe—C5	40.50 (14)	C5—C4—Fe	69.79 (18)
C3—Fe—C7	126.85 (12)	C3—C4—Fe	69.49 (17)
C4—Fe—C7	165.51 (13)	C5—C4—H4	126.2
C5—Fe—C7	152.17 (14)	C3—C4—H4	126.2
C3—Fe—C2	40.37 (13)	Fe—C4—H4	126.1
C4—Fe—C2	68.37 (13)	C1—C5—C4	108.4 (3)
C5—Fe—C2	68.20 (13)	C1—C5—Fe	69.99 (17)
C7—Fe—C2	107.11 (12)	C4—C5—Fe	69.71 (17)
C3—Fe—C8	107.68 (12)	C1—C5—H5	125.8
C4—Fe—C8	127.68 (13)	C4—C5—H5	125.8
C5—Fe—C8	165.74 (14)	Fe—C5—H5	126.1
C7—Fe—C8	41.13 (11)	C7—C6—C10	107.1 (2)
C2—Fe—C8	118.32 (13)	C7—C6—C11	126.9 (2)
C3—Fe—C1	68.17 (13)	C10—C6—C11	126.0 (2)
C4—Fe—C1	68.10 (14)	C7—C6—Fe	68.97 (15)
C5—Fe—C1	40.30 (14)	C10—C6—Fe	69.28 (15)
C7—Fe—C1	118.13 (13)	C11—C6—Fe	128.33 (19)
C2—Fe—C1	40.69 (13)	C6—C7—C8	108.0 (2)
C8—Fe—C1	152.45 (14)	C6—C7—Fe	70.09 (15)
C3—Fe—C10	153.13 (12)	C8—C7—Fe	69.56 (16)
C4—Fe—C10	119.09 (12)	C6—C7—H7	126.0
C5—Fe—C10	108.57 (12)	C8—C7—H7	126.0
C7—Fe—C10	68.70 (11)	Fe—C7—H7	125.9
C2—Fe—C10	165.43 (12)	C9—C8—C7	108.1 (2)
C8—Fe—C10	68.36 (12)	C9—C8—Fe	69.89 (16)
C1—Fe—C10	127.81 (13)	C7—C8—Fe	69.32 (15)
C3—Fe—C9	119.06 (12)	C9—C8—H8	126.0
C4—Fe—C9	108.37 (12)	C7—C8—H8	126.0
C5—Fe—C9	128.08 (13)	Fe—C8—H8	126.4
C7—Fe—C9	68.88 (11)	C10—C9—C8	108.0 (2)
C2—Fe—C9	152.56 (13)	C10—C9—Fe	69.72 (16)
C8—Fe—C9	40.70 (12)	C8—C9—Fe	69.41 (16)
C1—Fe—C9	165.56 (13)	C10—C9—H9	126.0
C10—Fe—C9	40.48 (11)	C8—C9—H9	126.0
C3—Fe—C6	164.67 (12)	Fe—C9—H9	126.5

C4—Fe—C6	152.67 (12)	C9—C10—C6	108.7 (2)
C5—Fe—C6	118.56 (12)	C9—C10—Fe	69.81 (16)
C7—Fe—C6	40.94 (10)	C6—C10—Fe	69.77 (15)
C2—Fe—C6	126.92 (12)	C9—C10—H10	125.6
C8—Fe—C6	68.94 (11)	C6—C10—H10	125.6
C1—Fe—C6	107.50 (12)	Fe—C10—H10	126.4
C10—Fe—C6	40.95 (11)	C12—C11—C16	117.9 (3)
C9—Fe—C6	68.80 (11)	C12—C11—C6	121.3 (2)
C5—C1—C2	108.1 (3)	C16—C11—C6	120.8 (3)
C5—C1—Fe	69.70 (18)	C11—C12—C13	121.2 (3)
C2—C1—Fe	69.60 (17)	C11—C12—H12	119.4
C5—C1—H1	126.0	C13—C12—H12	119.4
C2—C1—H1	126.0	C14—C13—C12	118.4 (3)
Fe—C1—H1	126.3	C14—C13—H13	120.8
C3—C2—C1	107.9 (3)	C12—C13—H13	120.8
C3—C2—Fe	69.66 (17)	C15—C14—C13	121.9 (3)
C1—C2—Fe	69.71 (17)	C15—C14—Br	119.2 (2)
C3—C2—H2	126.0	C13—C14—Br	118.9 (2)
C1—C2—H2	126.0	C14—C15—C16	119.0 (3)
Fe—C2—H2	126.2	C14—C15—H15	120.5
C2—C3—C4	108.0 (3)	C16—C15—H15	120.5
C2—C3—Fe	69.96 (17)	C15—C16—C11	121.5 (3)
C4—C3—Fe	69.53 (17)	C15—C16—H16	119.2
C2—C3—H3	126.0	C11—C16—H16	119.2
C4—C3—H3	126.0		
C3—Fe—C1—C5	−81.8 (2)	C9—Fe—C6—C10	37.07 (17)
C4—Fe—C1—C5	−37.5 (2)	C3—Fe—C6—C11	−79.1 (5)
C7—Fe—C1—C5	156.93 (19)	C4—Fe—C6—C11	68.0 (4)
C2—Fe—C1—C5	−119.4 (3)	C5—Fe—C6—C11	34.3 (3)
C8—Fe—C1—C5	−168.4 (2)	C7—Fe—C6—C11	−121.0 (3)
C10—Fe—C1—C5	73.0 (2)	C2—Fe—C6—C11	−48.8 (3)
C9—Fe—C1—C5	41.0 (6)	C8—Fe—C6—C11	−159.0 (3)
C6—Fe—C1—C5	113.8 (2)	C1—Fe—C6—C11	−8.0 (3)
C3—Fe—C1—C2	37.54 (19)	C10—Fe—C6—C11	120.1 (3)
C4—Fe—C1—C2	81.9 (2)	C9—Fe—C6—C11	157.2 (3)
C5—Fe—C1—C2	119.4 (3)	C10—C6—C7—C8	0.4 (3)
C7—Fe—C1—C2	−83.7 (2)	C11—C6—C7—C8	−177.7 (2)
C8—Fe—C1—C2	−49.0 (3)	Fe—C6—C7—C8	59.43 (19)
C10—Fe—C1—C2	−167.57 (17)	C10—C6—C7—Fe	−59.00 (18)
C9—Fe—C1—C2	160.4 (4)	C11—C6—C7—Fe	122.8 (3)
C6—Fe—C1—C2	−126.84 (18)	C3—Fe—C7—C6	−167.24 (17)
C5—C1—C2—C3	−0.1 (3)	C4—Fe—C7—C6	163.3 (4)
Fe—C1—C2—C3	−59.4 (2)	C5—Fe—C7—C6	−51.6 (3)
C5—C1—C2—Fe	59.3 (2)	C2—Fe—C7—C6	−127.18 (17)
C4—Fe—C2—C3	38.05 (19)	C8—Fe—C7—C6	119.1 (2)
C5—Fe—C2—C3	81.8 (2)	C1—Fe—C7—C6	−84.50 (19)
C7—Fe—C2—C3	−127.35 (18)	C10—Fe—C7—C6	38.03 (16)
C8—Fe—C2—C3	−84.2 (2)	C9—Fe—C7—C6	81.59 (17)
C1—Fe—C2—C3	119.2 (3)	C3—Fe—C7—C8	73.7 (2)

C10—Fe—C2—C3	161.7 (4)	C4—Fe—C7—C8	44.2 (5)
C9—Fe—C2—C3	−50.4 (3)	C5—Fe—C7—C8	−170.7 (2)
C6—Fe—C2—C3	−168.12 (17)	C2—Fe—C7—C8	113.71 (18)
C3—Fe—C2—C1	−119.2 (3)	C1—Fe—C7—C8	156.39 (18)
C4—Fe—C2—C1	−81.1 (2)	C10—Fe—C7—C8	−81.08 (18)
C5—Fe—C2—C1	−37.4 (2)	C9—Fe—C7—C8	−37.51 (17)
C7—Fe—C2—C1	113.5 (2)	C6—Fe—C7—C8	−119.1 (2)
C8—Fe—C2—C1	156.65 (19)	C6—C7—C8—C9	−0.4 (3)
C10—Fe—C2—C1	42.5 (5)	Fe—C7—C8—C9	59.35 (19)
C9—Fe—C2—C1	−169.5 (2)	C6—C7—C8—Fe	−59.76 (18)
C6—Fe—C2—C1	72.7 (2)	C3—Fe—C8—C9	114.28 (18)
C1—C2—C3—C4	0.0 (3)	C4—Fe—C8—C9	73.3 (2)
Fe—C2—C3—C4	−59.4 (2)	C5—Fe—C8—C9	42.8 (6)
C1—C2—C3—Fe	59.4 (2)	C7—Fe—C8—C9	−119.4 (2)
C4—Fe—C3—C2	−119.1 (3)	C2—Fe—C8—C9	156.84 (17)
C5—Fe—C3—C2	−81.4 (2)	C1—Fe—C8—C9	−169.2 (2)
C7—Fe—C3—C2	71.7 (2)	C10—Fe—C8—C9	−37.46 (16)
C8—Fe—C3—C2	113.20 (19)	C6—Fe—C8—C9	−81.58 (18)
C1—Fe—C3—C2	−37.82 (19)	C3—Fe—C8—C7	−126.30 (17)
C10—Fe—C3—C2	−169.9 (2)	C4—Fe—C8—C7	−167.27 (17)
C9—Fe—C3—C2	156.04 (18)	C5—Fe—C8—C7	162.2 (5)
C6—Fe—C3—C2	38.5 (5)	C2—Fe—C8—C7	−83.74 (19)
C5—Fe—C3—C4	37.7 (2)	C1—Fe—C8—C7	−49.8 (3)
C7—Fe—C3—C4	−169.18 (18)	C10—Fe—C8—C7	81.96 (17)
C2—Fe—C3—C4	119.1 (3)	C9—Fe—C8—C7	119.4 (2)
C8—Fe—C3—C4	−127.70 (19)	C6—Fe—C8—C7	37.84 (16)
C1—Fe—C3—C4	81.3 (2)	C7—C8—C9—C10	0.2 (3)
C10—Fe—C3—C4	−50.8 (3)	Fe—C8—C9—C10	59.22 (19)
C9—Fe—C3—C4	−84.9 (2)	C7—C8—C9—Fe	−59.00 (19)
C6—Fe—C3—C4	157.6 (4)	C3—Fe—C9—C10	157.07 (17)
C2—C3—C4—C5	0.0 (3)	C4—Fe—C9—C10	113.59 (18)
Fe—C3—C4—C5	−59.6 (2)	C5—Fe—C9—C10	72.8 (2)
C2—C3—C4—Fe	59.6 (2)	C7—Fe—C9—C10	−81.54 (17)
C3—Fe—C4—C5	118.8 (3)	C2—Fe—C9—C10	−168.1 (2)
C7—Fe—C4—C5	155.7 (4)	C8—Fe—C9—C10	−119.4 (2)
C2—Fe—C4—C5	81.3 (2)	C1—Fe—C9—C10	40.2 (6)
C8—Fe—C4—C5	−168.89 (19)	C6—Fe—C9—C10	−37.49 (16)
C1—Fe—C4—C5	37.35 (19)	C3—Fe—C9—C8	−83.5 (2)
C10—Fe—C4—C5	−84.8 (2)	C4—Fe—C9—C8	−126.99 (18)
C9—Fe—C4—C5	−127.73 (19)	C5—Fe—C9—C8	−167.72 (18)
C6—Fe—C4—C5	−48.5 (3)	C7—Fe—C9—C8	37.89 (16)
C5—Fe—C4—C3	−118.8 (3)	C2—Fe—C9—C8	−48.7 (3)
C7—Fe—C4—C3	36.9 (6)	C1—Fe—C9—C8	159.7 (5)
C2—Fe—C4—C3	−37.50 (18)	C10—Fe—C9—C8	119.4 (2)
C8—Fe—C4—C3	72.3 (2)	C6—Fe—C9—C8	81.94 (17)
C1—Fe—C4—C3	−81.5 (2)	C8—C9—C10—C6	0.0 (3)
C10—Fe—C4—C3	156.36 (18)	Fe—C9—C10—C6	59.08 (19)
C9—Fe—C4—C3	113.45 (19)	C8—C9—C10—Fe	−59.03 (19)
C6—Fe—C4—C3	−167.3 (2)	C7—C6—C10—C9	−0.3 (3)

C2—C1—C5—C4	0.1 (3)	C11—C6—C10—C9	177.9 (2)
Fe—C1—C5—C4	59.3 (2)	Fe—C6—C10—C9	−59.10 (19)
C2—C1—C5—Fe	−59.2 (2)	C7—C6—C10—Fe	58.80 (18)
C3—C4—C5—C1	−0.1 (3)	C11—C6—C10—Fe	−123.0 (3)
Fe—C4—C5—C1	−59.5 (2)	C3—Fe—C10—C9	−48.9 (3)
C3—C4—C5—Fe	59.4 (2)	C4—Fe—C10—C9	−84.5 (2)
C3—Fe—C5—C1	81.3 (2)	C5—Fe—C10—C9	−127.49 (19)
C4—Fe—C5—C1	119.5 (3)	C7—Fe—C10—C9	82.01 (18)
C7—Fe—C5—C1	−47.8 (3)	C2—Fe—C10—C9	157.9 (4)
C2—Fe—C5—C1	37.72 (19)	C8—Fe—C10—C9	37.67 (17)
C8—Fe—C5—C1	157.7 (5)	C1—Fe—C10—C9	−168.24 (18)
C10—Fe—C5—C1	−127.14 (19)	C6—Fe—C10—C9	120.0 (2)
C9—Fe—C5—C1	−168.01 (18)	C3—Fe—C10—C6	−168.9 (2)
C6—Fe—C5—C1	−83.5 (2)	C4—Fe—C10—C6	155.50 (17)
C3—Fe—C5—C4	−38.18 (19)	C5—Fe—C10—C6	112.47 (18)
C7—Fe—C5—C4	−167.3 (2)	C7—Fe—C10—C6	−38.02 (16)
C2—Fe—C5—C4	−81.8 (2)	C2—Fe—C10—C6	37.8 (5)
C8—Fe—C5—C4	38.2 (6)	C8—Fe—C10—C6	−82.37 (17)
C1—Fe—C5—C4	−119.5 (3)	C1—Fe—C10—C6	71.7 (2)
C10—Fe—C5—C4	113.35 (19)	C9—Fe—C10—C6	−120.0 (2)
C9—Fe—C5—C4	72.5 (2)	C7—C6—C11—C12	−12.5 (4)
C6—Fe—C5—C4	156.95 (18)	C10—C6—C11—C12	169.7 (3)
C3—Fe—C6—C7	42.0 (5)	Fe—C6—C11—C12	78.7 (3)
C4—Fe—C6—C7	−171.0 (2)	C7—C6—C11—C16	165.4 (3)
C5—Fe—C6—C7	155.38 (18)	C10—C6—C11—C16	−12.4 (4)
C2—Fe—C6—C7	72.3 (2)	Fe—C6—C11—C16	−103.4 (3)
C8—Fe—C6—C7	−38.01 (16)	C16—C11—C12—C13	−1.1 (5)
C1—Fe—C6—C7	113.01 (18)	C6—C11—C12—C13	176.9 (3)
C10—Fe—C6—C7	−118.9 (2)	C11—C12—C13—C14	0.4 (5)
C9—Fe—C6—C7	−81.79 (17)	C12—C13—C14—C15	0.3 (5)
C3—Fe—C6—C10	160.8 (4)	C12—C13—C14—Br	−178.6 (2)
C4—Fe—C6—C10	−52.1 (3)	C13—C14—C15—C16	−0.3 (5)
C5—Fe—C6—C10	−85.8 (2)	Br—C14—C15—C16	178.6 (2)
C7—Fe—C6—C10	118.9 (2)	C14—C15—C16—C11	−0.4 (5)
C2—Fe—C6—C10	−168.88 (17)	C12—C11—C16—C15	1.0 (4)
C8—Fe—C6—C10	80.85 (18)	C6—C11—C16—C15	−176.9 (3)
C1—Fe—C6—C10	−128.13 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cg1^{i}	0.95	2.90	3.780 (4)	154

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2.

Fig. 1

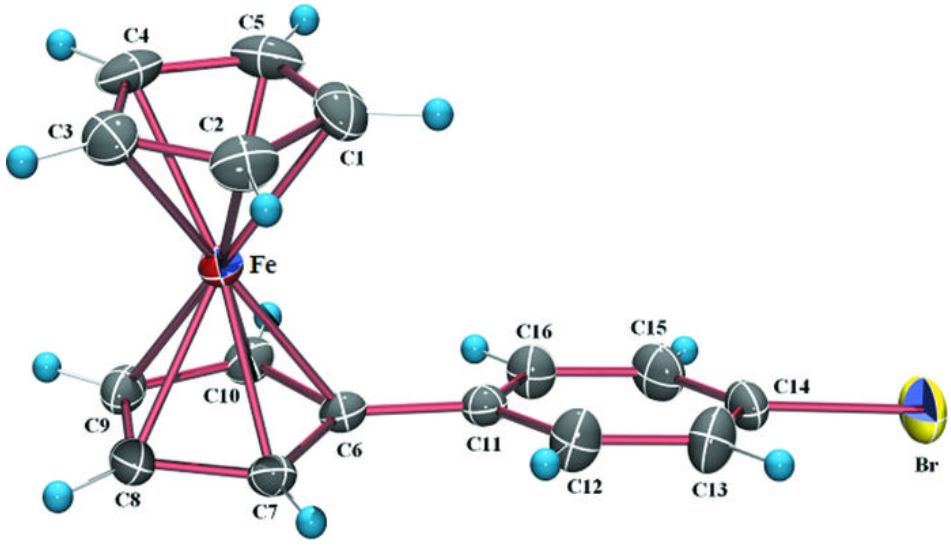


Fig. 2