Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

11-Bromo-1-ferrocenylundecan-1-one

C. John McAdam, Brian H. Robinson and Jim Simpson*

Department of Chemistry, University of Otago, PO Box 56, Dunedin, New Zealand
Correspondence e-mail: jsimpson@alkali.otago.ac.nz

Received 3 April 2007; accepted 3 April 2007

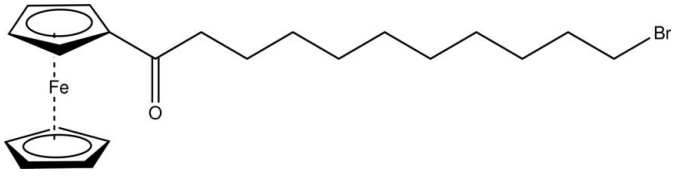
Key indicators: single-crystal X-ray study; T = 85 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.120; data-to-parameter ratio = 33.0.

In the title compound, [Fe(C_5H_5)($C_{16}H_{24}$BrO)], the η^5-cyclopentadiene rings are essentially eclipsed, while the well ordered chain of the undecanone substituent is bowed significantly towards the Fe atom. In the crystal structure, adjacent molecules form inversion-related dimers through weak C—H···O and C—H···Br interactions. These dimers are further aggregated by intermolecular C—H···π interactions between neighbouring cyclopentadiene rings, forming zigzag chains along the c axis.

Related literature

The longest methylene chain to have been examined crystallographically (Cambridge Structural Database, Version 5.28, 2007; Allen, 2002) for a similar ferrocenyl compound is 6-bromohexanoylferrocene (Hursthouse *et al.*, 2003), while that in an organic compound is for 1-(4-*tert*-butylphenyl)-4-chlorobutan-1-one (Anilkumar *et al.*, 2005). A 1,6-diferrocenylhexane-1,6-dione has also been reported (Pugh *et al.*, 2004).

For related literature, see: McAdam *et al.* (2000).



Experimental

Crystal data

[Fe(C_5H_5)($C_{15}H_{24}$BrO)]
M_r = 433.20
Monoclinic, $P2_1/c$
a = 5.6027 (2) Å
b = 9.8858 (4) Å
c = 35.0048 (15) Å
β = 92.576 (2)°
V = 1936.86 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.85 mm^{-1}
T = 85 (2) K
0.53 × 0.12 × 0.03 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.700, T_{max} = 0.918
37380 measured reflections
7152 independent reflections
5902 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.120
S = 1.22
7152 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −2.43 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17···Br1^{i}	0.95	3.01	3.797 (3)	142
C1—H1B···O11^{i}	0.99	2.55	3.422 (3)	147
C14—H14···$Cg2^{ii}$	0.95	2.94	3.647 (3)	133

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+2, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997) and *TITAN2000* (Hunter & Simpson, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997) and *TITAN2000*; molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*, *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2003) and *PARST* (Nardelli, 1995).

The authors are grateful to students in the CHEM303 class of 2007 at the University of Otago for preparation of the title compound. We also thank the New Zealand Foundation for Research Science and Technology for a Postdoctoral Fellowship to CJM and the University of Otago for purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2360).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
Anilkumar, H. G., Vijay, T., Yathirajan, H. S., Narasimhamurthy, T. & Rathore, R. S. (2005). *Acta Cryst.* E**61**, o3332–o3333.
Bruker (2004). *APEX2* (Version 1.017), *SAINT* (Version 7.12a) and *SADABS* (Version 2004/1). Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Hunter, K. A. & Simpson, J. (1999). *TITAN2000*. University of Otago, New Zealand.
Hursthouse, M. B., Hibbs, D. E. & Butler, I. R. (2003). Private communication to the CCDC, refcode BAVBOQ.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
McAdam, C. J., Robinson, B. H. & Simpson, J. (2000). *Organometallics*, **19**, 3644–3653.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Pugh, C. A., Lufaso, M. W., Zeller, M., Wagner, T. R. & Curtin, L. S. (2004). *J. Organomet. Chem.* **691**, 680–686.
Saji, T., Hoshino, K., Ishii, Y. & Goto, M. (1991). *J. Am. Chem. Soc.* **113**, 450–456.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

  doi:10.1107/S1600536807016510

supplementary materials

Acta Cryst. (2007). E**63**, m1362 [**doi:10.1107/S1600536807016510**]

11-Bromo-1-ferrocenylundecan-1-one

C. J. McAdam, B. H. Robinson and J. Simpson

Comment

The title compound, (I), is a useful precursor for the preparation of amino ferrocenyl derivatives (McAdam *et al.*, 2000) or redox active surfactant systems (Saji *et al.*, 2000) and its structure is reported here (Fig. 1). The cyclopentadienyl rings of the ferrocene are approximately eclipsed, with a mean *Cm*—*Cg*1—*Cg*2—Cn torsion angle of 4.2 (2)° (*Cg*1 and *Cg*2 are the centroids of the cyclopentadienyl rings, m = 12–16 and n = 17–21). The dihedral angle between the Cp ring mean planes is 4.68 (15)°. The ten-membered methylene chain of the undecanone substituent is nicely ordered and is bowed significantly towards the Fe atom. While the C11 atom lies 0.070 (3) Å above the C12···C16 ring plane, atom C1 is 0.735 (5) Å below that plane in the direction of the Fe1 atom.

In the crystal structure molecules of (I) link in a head-to-tail fashion through C17—H17···Br1 and C1···H1B···O11 hydrogen bonds to form inversion related dimers (Fig 2, Table 1). Then, C14—H14···*Cg*2 interactions link the dimers into an extended zigzag chain along the *c* axis (Fig. 3).

Experimental

The title compound was prepared using the method of Saji *et al.* (1991). Yellow rectangular plates were grown by slow evaporation from a CH_2Cl_2–toluene (1:1 v/v) solvent system.

Refinement

All H atoms were positioned geometrically, with C—H = 0.95–0.99 Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

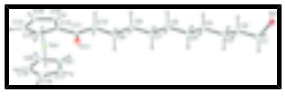


Fig. 1. The molecular structure of (I), with the atom-labelling scheme and 50% probability displacement ellipsoids.

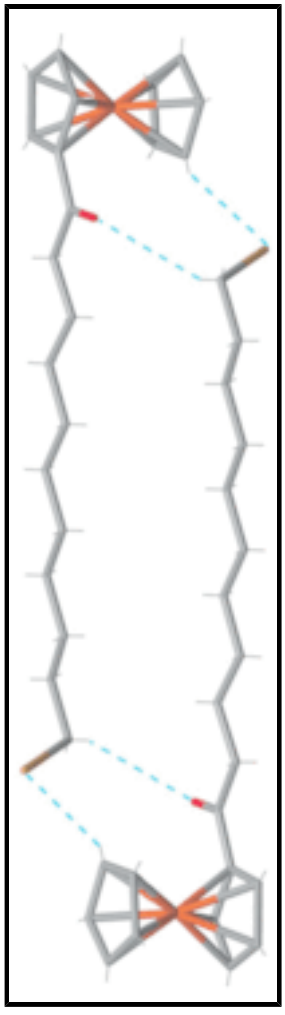


Fig. 2. Formation of inversion related dimers of (I) with hydrogen bonds drawn as dashed lines.

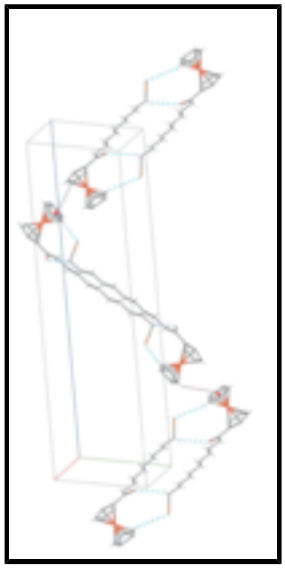


Fig. 3. Part of the packing of (I), with hydrogen bonds drawn as blue dashed lines and C—H···π interactions drawn as purple dashed lines. The red circles represent centroids of the C18···C21 rings.

11-Bromo-1-ferrocenylundecan-1-one

Crystal data

$[Fe(C_5H_5)(C_{15}H_{24}BrO)]$	$F_{000} = 896$
$M_r = 433.20$	$D_x = 1.486$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 6638 reflections
$a = 5.6027$ (2) Å	$\theta = 2.4$–32.0^o
$b = 9.8858$ (4) Å	$\mu = 2.85$ mm^{-1}
$c = 35.0048$ (15) Å	$T = 85$ (2) K
$\beta = 92.576$ (2)^o	Rectangular plate, yellow
$V = 1936.86$ (13) Å^3	0.53 × 0.12 × 0.03 mm
$Z = 4$	

Data collection

Bruker APEXII CCD area-detector diffractometer	7152 independent reflections
Radiation source: fine-focus sealed tube	5902 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.041$
$T = 85(2)$ K	$\theta_{max} = 34.7^o$
φ and ω scans	$\theta_{min} = 1.2^o$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -8 \rightarrow 8$
$T_{min} = 0.700$, $T_{max} = 0.918$	$k = -15 \rightarrow 14$
37380 measured reflections	$l = -52 \rightarrow 53$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 2.8882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.050$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.120$	$\Delta\rho_{max} = 0.97$ e Å^{-3}
$S = 1.22$	$\Delta\rho_{min} = -2.43$ e Å^{-3}
7152 reflections	Extinction correction: none
217 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br1	0.44415 (5)	0.29956 (3)	0.174591 (8)	0.02083 (8)
C1	0.6436 (5)	0.2608 (3)	0.13114 (7)	0.0179 (5)
H1A	0.8027	0.2291	0.1408	0.022*
H1B	0.5691	0.1874	0.1155	0.022*
C2	0.6732 (5)	0.3844 (2)	0.10645 (7)	0.0168 (5)
H2A	0.7894	0.3630	0.0868	0.020*
H2B	0.7425	0.4579	0.1226	0.020*
C3	0.4447 (5)	0.4366 (3)	0.08631 (8)	0.0186 (5)
H3A	0.3292	0.4610	0.1058	0.022*
H3B	0.3729	0.3633	0.0703	0.022*
C4	0.4869 (5)	0.5596 (3)	0.06113 (8)	0.0198 (5)
H4A	0.5480	0.6347	0.0775	0.024*
H4B	0.6119	0.5370	0.0431	0.024*
C5	0.2652 (5)	0.6077 (3)	0.03841 (8)	0.0191 (5)
H5A	0.1404	0.6312	0.0564	0.023*
H5B	0.2033	0.5326	0.0221	0.023*
C6	0.3113 (5)	0.7300 (3)	0.01325 (8)	0.0184 (5)
H6A	0.3603	0.8072	0.0298	0.022*
H6B	0.4458	0.7090	−0.0032	0.022*
C7	0.0957 (5)	0.7721 (3)	−0.01212 (7)	0.0177 (5)
H7A	−0.0379	0.7950	0.0043	0.021*
H7B	0.0446	0.6945	−0.0284	0.021*
C8	0.1459 (5)	0.8929 (3)	−0.03771 (7)	0.0159 (4)
H8A	0.2858	0.8718	−0.0530	0.019*
H8B	0.1879	0.9719	−0.0214	0.019*
C9	−0.0648 (5)	0.9311 (3)	−0.06499 (7)	0.0167 (5)
H9A	−0.1051	0.8533	−0.0819	0.020*
H9B	−0.2060	0.9513	−0.0500	0.020*
C10	−0.0073 (4)	1.0539 (2)	−0.08942 (7)	0.0146 (4)
H10A	0.0461	1.1287	−0.0723	0.017*
H10B	0.1274	1.0306	−0.1056	0.017*
C11	−0.2143 (4)	1.1037 (2)	−0.11510 (7)	0.0126 (4)
O11	−0.4154 (3)	1.0556 (2)	−0.11395 (6)	0.0190 (4)

C12	−0.1618 (4)	1.2151 (2)	−0.14154 (7)	0.0112 (4)
C13	−0.3250 (4)	1.2695 (2)	−0.17037 (7)	0.0129 (4)
H13	−0.4880	1.2448	−0.1745	0.015*
C14	−0.1994 (5)	1.3668 (2)	−0.19158 (7)	0.0151 (4)
H14	−0.2645	1.4185	−0.2124	0.018*
C15	0.0394 (5)	1.3739 (2)	−0.17642 (7)	0.0143 (4)
H15	0.1610	1.4313	−0.1853	0.017*
C16	0.0661 (4)	1.2797 (2)	−0.14536 (7)	0.0131 (4)
H16	0.2078	1.2631	−0.1301	0.016*
Fe1	−0.03768 (6)	1.18054 (3)	−0.194497 (9)	0.00942 (8)
C17	−0.0130 (4)	0.9752 (2)	−0.20303 (8)	0.0157 (4)
H17	−0.0588	0.9063	−0.1859	0.019*
C18	−0.1625 (4)	1.0354 (3)	−0.23260 (7)	0.0159 (4)
H18	−0.3248	1.0132	−0.2386	0.019*
C19	−0.0246 (4)	1.1347 (3)	−0.25143 (7)	0.0154 (4)
H19	−0.0794	1.1904	−0.2721	0.018*
C20	0.2096 (4)	1.1356 (3)	−0.23371 (7)	0.0146 (4)
H20	0.3382	1.1919	−0.2406	0.018*
C21	0.2170 (4)	1.0369 (2)	−0.20378 (7)	0.0148 (4)
H21	0.3514	1.0160	−0.1873	0.018*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02858 (15)	0.01801 (13)	0.01621 (13)	0.00177 (10)	0.00468 (10)	0.00173 (9)
C1	0.0245 (12)	0.0152 (11)	0.0143 (11)	0.0046 (9)	0.0026 (9)	0.0018 (9)
C2	0.0224 (12)	0.0128 (10)	0.0153 (11)	0.0012 (9)	0.0002 (9)	0.0025 (8)
C3	0.0226 (12)	0.0162 (11)	0.0166 (12)	−0.0005 (9)	−0.0028 (9)	0.0043 (9)
C4	0.0249 (13)	0.0178 (11)	0.0163 (12)	0.0011 (10)	−0.0037 (10)	0.0047 (9)
C5	0.0236 (12)	0.0161 (11)	0.0172 (12)	−0.0001 (9)	−0.0022 (10)	0.0044 (9)
C6	0.0248 (13)	0.0139 (11)	0.0163 (12)	0.0016 (9)	−0.0022 (10)	0.0035 (9)
C7	0.0234 (12)	0.0158 (11)	0.0140 (11)	0.0022 (9)	0.0005 (9)	0.0046 (9)
C8	0.0192 (11)	0.0149 (10)	0.0134 (11)	0.0027 (8)	−0.0010 (9)	0.0027 (8)
C9	0.0202 (11)	0.0148 (10)	0.0155 (11)	−0.0002 (9)	0.0034 (9)	0.0044 (9)
C10	0.0160 (10)	0.0153 (10)	0.0124 (10)	−0.0008 (8)	0.0007 (8)	0.0028 (8)
C11	0.0149 (10)	0.0125 (10)	0.0106 (10)	0.0014 (8)	0.0028 (8)	0.0004 (8)
O11	0.0142 (8)	0.0210 (9)	0.0218 (9)	−0.0029 (7)	0.0019 (7)	0.0068 (7)
C12	0.0134 (9)	0.0099 (9)	0.0103 (10)	0.0005 (7)	0.0013 (8)	−0.0002 (7)
C13	0.0137 (10)	0.0116 (10)	0.0133 (10)	0.0033 (8)	0.0008 (8)	−0.0001 (8)
C14	0.0216 (12)	0.0098 (9)	0.0138 (11)	0.0039 (8)	0.0006 (9)	0.0013 (8)
C15	0.0202 (11)	0.0104 (9)	0.0126 (10)	−0.0026 (8)	0.0031 (9)	−0.0013 (8)
C16	0.0169 (10)	0.0113 (9)	0.0108 (10)	−0.0019 (8)	−0.0003 (8)	−0.0011 (8)
Fe1	0.01107 (14)	0.00823 (14)	0.00895 (15)	0.00050 (11)	0.00024 (11)	−0.00029 (11)
C17	0.0162 (11)	0.0104 (10)	0.0207 (12)	0.0016 (8)	0.0010 (9)	−0.0034 (9)
C18	0.0130 (10)	0.0162 (11)	0.0184 (11)	−0.0012 (8)	0.0009 (8)	−0.0072 (9)
C19	0.0171 (11)	0.0186 (11)	0.0105 (10)	0.0029 (9)	0.0004 (8)	−0.0022 (8)
C20	0.0149 (10)	0.0155 (10)	0.0137 (11)	0.0013 (8)	0.0037 (8)	−0.0019 (8)
C21	0.0145 (10)	0.0133 (10)	0.0168 (11)	0.0032 (8)	0.0022 (8)	−0.0012 (8)

Geometric parameters (Å, °)

Br1—C1	1.965 (3)	C11—O11	1.225 (3)
C1—C2	1.511 (3)	C11—C12	1.477 (3)
C1—H1A	0.9900	C12—C13	1.436 (3)
C1—H1B	0.9900	C12—C16	1.439 (3)
C2—C3	1.523 (4)	C12—Fe1	2.038 (2)
C2—H2A	0.9900	C13—C14	1.421 (3)
C2—H2B	0.9900	C13—Fe1	2.050 (2)
C3—C4	1.526 (4)	C13—H13	0.9500
C3—H3A	0.9900	C14—C15	1.419 (4)
C3—H3B	0.9900	C14—Fe1	2.057 (2)
C4—C5	1.521 (4)	C14—H14	0.9500
C4—H4A	0.9900	C15—C16	1.434 (3)
C4—H4B	0.9900	C15—Fe1	2.053 (2)
C5—C6	1.525 (4)	C15—H15	0.9500
C5—H5A	0.9900	C16—Fe1	2.042 (2)
C5—H5B	0.9900	C16—H16	0.9500
C6—C7	1.525 (4)	Fe1—C20	2.042 (2)
C6—H6A	0.9900	Fe1—C19	2.048 (2)
C6—H6B	0.9900	Fe1—C21	2.050 (2)
C7—C8	1.527 (3)	Fe1—C17	2.057 (2)
C7—H7A	0.9900	Fe1—C18	2.060 (2)
C7—H7B	0.9900	C17—C21	1.427 (3)
C8—C9	1.532 (4)	C17—C18	1.432 (4)
C8—H8A	0.9900	C17—H17	0.9500
C8—H8B	0.9900	C18—C19	1.428 (4)
C9—C10	1.528 (3)	C18—H18	0.9500
C9—H9A	0.9900	C19—C20	1.426 (4)
C9—H9B	0.9900	C19—H19	0.9500
C10—C11	1.517 (3)	C20—C21	1.431 (3)
C10—H10A	0.9900	C20—H20	0.9500
C10—H10B	0.9900	C21—H21	0.9500
C2—C1—Br1	111.46 (17)	C14—C15—H15	125.8
C2—C1—H1A	109.3	C16—C15—H15	125.8
Br1—C1—H1A	109.3	Fe1—C15—H15	126.8
C2—C1—H1B	109.3	C15—C16—C12	107.2 (2)
Br1—C1—H1B	109.3	C15—C16—Fe1	69.94 (14)
H1A—C1—H1B	108.0	C12—C16—Fe1	69.19 (13)
C1—C2—C3	115.3 (2)	C15—C16—H16	126.4
C1—C2—H2A	108.5	C12—C16—H16	126.4
C3—C2—H2A	108.5	Fe1—C16—H16	126.0
C1—C2—H2B	108.5	C12—Fe1—C16	41.32 (9)
C3—C2—H2B	108.5	C12—Fe1—C20	156.54 (10)
H2A—C2—H2B	107.5	C16—Fe1—C20	119.64 (10)
C2—C3—C4	112.9 (2)	C12—Fe1—C19	161.95 (10)
C2—C3—H3A	109.0	C16—Fe1—C19	154.77 (10)
C4—C3—H3A	109.0	C20—Fe1—C19	40.80 (10)

C2—C3—H3B	109.0	C12—Fe1—C13	41.13 (9)
C4—C3—H3B	109.0	C16—Fe1—C13	69.27 (10)
H3A—C3—H3B	107.8	C20—Fe1—C13	159.94 (10)
C5—C4—C3	114.0 (2)	C19—Fe1—C13	123.98 (10)
C5—C4—H4A	108.7	C12—Fe1—C21	121.93 (10)
C3—C4—H4A	108.7	C16—Fe1—C21	107.01 (10)
C5—C4—H4B	108.7	C20—Fe1—C21	40.95 (10)
C3—C4—H4B	108.7	C19—Fe1—C21	68.70 (10)
H4A—C4—H4B	107.6	C13—Fe1—C21	158.13 (10)
C4—C5—C6	113.2 (2)	C12—Fe1—C15	68.85 (9)
C4—C5—H5A	108.9	C16—Fe1—C15	41.00 (9)
C6—C5—H5A	108.9	C20—Fe1—C15	105.66 (10)
C4—C5—H5B	108.9	C19—Fe1—C15	119.31 (10)
C6—C5—H5B	108.9	C13—Fe1—C15	68.40 (10)
H5A—C5—H5B	107.7	C21—Fe1—C15	123.76 (10)
C7—C6—C5	113.7 (2)	C12—Fe1—C14	68.63 (9)
C7—C6—H6A	108.8	C16—Fe1—C14	68.75 (10)
C5—C6—H6A	108.8	C20—Fe1—C14	122.80 (10)
C7—C6—H6B	108.8	C19—Fe1—C14	106.35 (10)
C5—C6—H6B	108.8	C13—Fe1—C14	40.49 (10)
H6A—C6—H6B	107.7	C21—Fe1—C14	160.00 (10)
C6—C7—C8	113.1 (2)	C15—Fe1—C14	40.38 (10)
C6—C7—H7A	109.0	C12—Fe1—C17	108.99 (10)
C8—C7—H7A	109.0	C16—Fe1—C17	125.29 (10)
C6—C7—H7B	109.0	C20—Fe1—C17	68.64 (10)
C8—C7—H7B	109.0	C19—Fe1—C17	68.59 (10)
H7A—C7—H7B	107.8	C13—Fe1—C17	122.84 (10)
C7—C8—C9	113.7 (2)	C21—Fe1—C17	40.65 (10)
C7—C8—H8A	108.8	C15—Fe1—C17	161.56 (10)
C9—C8—H8A	108.8	C14—Fe1—C17	157.40 (10)
C7—C8—H8B	108.8	C12—Fe1—C18	125.88 (10)
C9—C8—H8B	108.8	C16—Fe1—C18	162.88 (10)
H8A—C8—H8B	107.7	C20—Fe1—C18	68.53 (10)
C10—C9—C8	111.6 (2)	C19—Fe1—C18	40.69 (10)
C10—C9—H9A	109.3	C13—Fe1—C18	108.40 (10)
C8—C9—H9A	109.3	C21—Fe1—C18	68.47 (10)
C10—C9—H9B	109.3	C15—Fe1—C18	155.31 (10)
C8—C9—H9B	109.3	C14—Fe1—C18	121.22 (10)
H9A—C9—H9B	108.0	C17—Fe1—C18	40.69 (10)
C11—C10—C9	114.5 (2)	C21—C17—C18	108.0 (2)
C11—C10—H10A	108.6	C21—C17—Fe1	69.38 (14)
C9—C10—H10A	108.6	C18—C17—Fe1	69.75 (14)
C11—C10—H10B	108.6	C21—C17—H17	126.0
C9—C10—H10B	108.6	C18—C17—H17	126.0
H10A—C10—H10B	107.6	Fe1—C17—H17	126.4
O11—C11—C12	121.3 (2)	C19—C18—C17	108.0 (2)
O11—C11—C10	122.3 (2)	C19—C18—Fe1	69.22 (14)
C12—C11—C10	116.4 (2)	C17—C18—Fe1	69.56 (14)
C13—C12—C16	108.0 (2)	C19—C18—H18	126.0

C13—C12—C11	125.5 (2)	C17—C18—H18	126.0
C16—C12—C11	126.3 (2)	Fe1—C18—H18	126.8
C13—C12—Fe1	69.88 (13)	C20—C19—C18	108.0 (2)
C16—C12—Fe1	69.49 (13)	C20—C19—Fe1	69.38 (14)
C11—C12—Fe1	122.06 (16)	C18—C19—Fe1	70.09 (14)
C14—C13—C12	107.8 (2)	C20—C19—H19	126.0
C14—C13—Fe1	70.03 (14)	C18—C19—H19	126.0
C12—C13—Fe1	68.99 (13)	Fe1—C19—H19	126.1
C14—C13—H13	126.1	C19—C20—C21	108.1 (2)
C12—C13—H13	126.1	C19—C20—Fe1	69.83 (14)
Fe1—C13—H13	126.5	C21—C20—Fe1	69.80 (14)
C15—C14—C13	108.6 (2)	C19—C20—H20	126.0
C15—C14—Fe1	69.68 (14)	C21—C20—H20	126.0
C13—C14—Fe1	69.48 (13)	Fe1—C20—H20	126.0
C15—C14—H14	125.7	C17—C21—C20	108.0 (2)
C13—C14—H14	125.7	C17—C21—Fe1	69.97 (13)
Fe1—C14—H14	126.7	C20—C21—Fe1	69.26 (13)
C14—C15—C16	108.4 (2)	C17—C21—H21	126.0
C14—C15—Fe1	69.94 (14)	C20—C21—H21	126.0
C16—C15—Fe1	69.06 (13)	Fe1—C21—H21	126.3

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C17—H17···Br1^{i}	0.95	3.01	3.797 (3)	142
C1—H1B···O11^{i}	0.99	2.55	3.422 (3)	147
C14—H14···Cg2^{ii}	0.95	2.94	3.647 (3)	133

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

Fig. 1

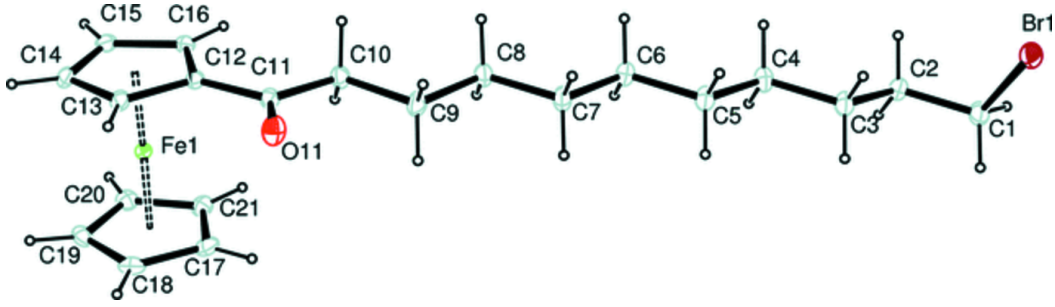

C15
C16
C14
C12
C11
C10
C8
C6
C4
C2
Br1
C13
C9
C7
C5
C3
C1
Fe1
O11
C20
C21
C19
C17
C18

Fig. 2

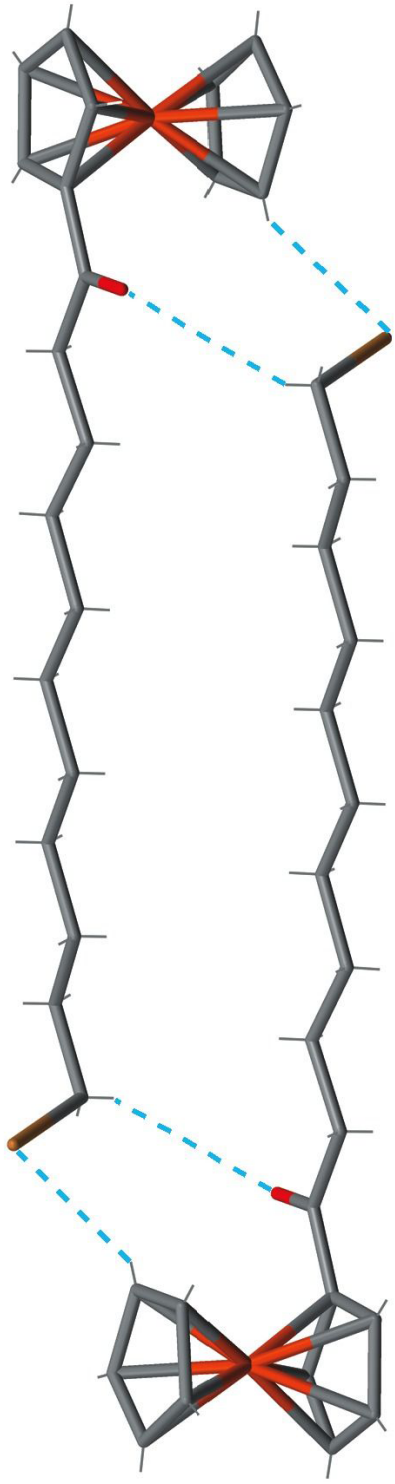


Fig. 3