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trans-1,2-Diferrocenyl-1,2-difluoroethene

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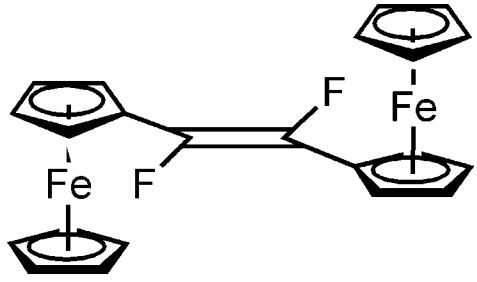
Key indicators: single-crystal X-ray study; T = 103 K; mean σ(C–C) = 0.004 Å; R factor = 0.035; wR factor = 0.067; data-to-parameter ratio = 12.6.

In the title compound, $[Fe_2(C_5H_5)_2(C_6H_4F)_2]$, the two fluoro and ferrocenyl groups are oriented in a *trans* arrangement as a result of crystallographic inversion symmetry. The C—F and C—C distances of the ethene framework are 1.365 (3) and 1.331 (5) Å, respectively.

Related literature

For related literature, see: Chen *et al.* (2000); Denifl *et al.* (1996); Lentz *et al.* (2004); Nagahora *et al.* (2004); Skibar *et al.* (2004).



Experimental

Crystal data

$[Fe_2(C_5H_5)_2(C_6H_4F)_2]$
M_r = 432.06
Tetragonal, $P4_2/n$
a = 16.968 (6) Å
c = 5.8668 (17) Å
V = 1689.2 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.74 mm^{-1}
T = 103 (2) K
0.30 × 0.10 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*REQAB*; Jacobson, 1998)
T_{min} = 0.623, T_{max} = 0.845
10691 measured reflections
1483 independent reflections
1361 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.067
S = 1.22
1483 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *yadokari-XG* (Wakita, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2164).

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supplementary materials

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trans-1,2-Diferrocenyl-1,2-difluoroethene

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Comment

Although a number of synthetic works on ferrocenyl substituted ethenes have been reported, only three reports are known for the crystalline structures of *trans*-1,2-diferrocenylethene derivatives, that is, *trans*-1,2-diferrocenylethene (Denifl *et al.*, 1996), *trans*-1,2-diferrocenyl-1,2-dimethylethene (Chen *et al.*, 2000), and *trans*-1,2-diferrocenyl-1,2-diphenylethene (Skibar *et al.*, 2004). During our course of studies on the syntheses of new π-conjugated compounds bearing ferrocenyl groups (Nagahora *et al.*, 2004), the crystal structure of *trans*-1,2-diferrocenyl-1,2-difluoroethene has been revealed.

The title compound was synthesized in 6% yield by the treatment of ferrocenyllithium, which was prepared by the reaction of ferrocene with *tert*-butyllithium, with 1,2-dibromo-1,1,2,2-tetrafluoroethane. The molecular structure of the title compound is shown in Fig. 1. It was found that two fluoro and ferrocenyl groups are located as *trans* configuration, respectively, with respect to the ethene framework. It has a center of symmetry in the middle of the C1—C1^{i} bond. The C1—C1^{i} and C1—C2 bond lengths (1.331 (5) and 1.448 (2) Å) of the title compound are in the range of those for the previously reported *trans*-Fc(*R*)C=C(*R*)Fc (Fc = ferrocenyl) (1.17 (1) and 1.47 (6) Å for *R* = H, 1.354 (4) and 1.517 (3) Å for *R* = Me, 1.29 (4) and 1.51 Å for *R* = Ph). The F1—C1 distance (1.365 (3) Å) is similar to that of *trans*-F(H)C=C(H)F (1.1349 (1) Å) (Lentz *et al.*, 2004). The dihedral angle between the least squares of C2—C3—C4—C5—C6 and C2^{i}—C3^{i}—C4^{i}—C5^{i}—C6^{i} (the cyclopentadienyl rings) is 18.6°, which is similar to that of the reported *trans*-Fc(H)C=C(H)Fc (15.1°). The shortest intermolecular contacts were found to be F1—H1^{iii} (2.4885 (15) Å) and F1—F1^{ii} (2.704 (2) Å), which are shorter than the sum of van der Waals radii between fluoro and hydrogen atoms (2.67 Å) and two fluoro atoms (2.94 Å), respectively (Fig. 2).

Experimental

A solution of *tert*-butyllithium in *n*-pentane (1.59 *M*; 17.3 ml, 27.5 mmol) was added to a THF (25 ml)/*n*-hexane (25 ml) solution of ferrocene (4.63 mg, 25.0 mmol) at 273 K. After stirring at the same temperature for 3 h, 1,2-dibromo-1,1,2,2-tetrafluoroethane (4.41 ml, 37.5 mmol) was added to the reaction mixture. After stirring at the same temperature for 1 h, the solution was allowed to be warmed up to room temperature for 12 h. After the removal of solvents, *n*-hexane was added to the residue and the mixture was filtered through Celite. The filtrate was purified by silica-gel column chromatography (eluting with *n*-hexane and chloroform) to afford the title compound (350 mg, 0.810 mmol, 5.9% based on the ferrocene) as an orange solid [m.p. 473 K (decomposition)]. Single crystals suitable for X-ray crystallographic analysis were obtained by slow recrystallization of its chloroform solution at room temperature.

Refinement

All H atoms were treated as riding with C—H distances of 0.95 Å, while all the other atoms were refined anisotropically.

Figures

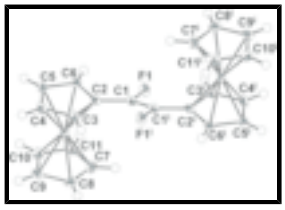


Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level [Symmetry code: (i) −*x*, 1 − *y*, −*z*.].

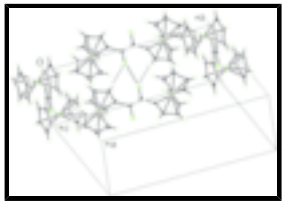


Fig. 2. The molecular packing of the title compound. Black dashed and gray solid lines indicate the F···F^{ii} and F···H^{iii} intramolecular contacts, respectively [Symmetry codes: (ii) −*x*, 1 − *y*, −1 − *z*; (iii) *x*, *y*, −1 + *z*.].

trans-1,2-Diferrocenyl-1,2-difluoroethene

Crystal data

$[Fe_2(C_5H_5)_2(C_6H_4F)_2]$	$Z = 4$
$M_r = 432.06$	$F_{000} = 880$
Tetragonal, $P4_2/n$	$D_x = 1.699$ Mg m^{-3}
Hall symbol: -P 4bc	Mo $K\alpha$ radiation $\lambda = 0.71070$ Å
$a = 16.968$ (6) Å	Cell parameters from 1483 reflections
$b = 16.968$ (6) Å	$\theta = 3.4$–25.0º
$c = 5.8668$ (17) Å	$\mu = 1.74$ mm^{-1}
$\alpha = 90$º	$T = 103$ (2) K
$\beta = 90$º	Needle, orange
$\gamma = 90$º	0.30 × 0.10 × 0.10 mm
$V = 1689.2$ (9) Å^3	

Data collection

Rigaku Mercury CCD diffractometer	1483 independent reflections
Radiation source: fine-focus sealed tube	1361 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.040$
Detector resolution: 7.31 pixels mm^{-1}	$\theta_{max} = 25.0$º
$T = 103(2)$ K	$\theta_{min} = 3.4$º
ω scans	$h = -20 \rightarrow 20$
Absorption correction: multi-scan (REQAB; Jacobson, 1998)	$k = -20 \rightarrow 19$
$T_{min} = 0.623$, $T_{max} = 0.845$	$l = -6 \rightarrow 6$
10691 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.067$	$w = 1/[\sigma^2(F_o^2) + (0.0205P)^2 + 1.7668P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.22$	$(\Delta/\sigma)_{max} = 0.001$
1483 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
118 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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}
Fe1	0.00676 (2)	0.71464 (2)	0.01662 (6)	0.01341 (13)
F1	0.01687 (9)	0.52552 (9)	−0.2872 (2)	0.0201 (4)
C1	0.01534 (15)	0.53068 (15)	−0.0550 (4)	0.0149 (5)
C2	0.05082 (15)	0.60226 (15)	0.0318 (4)	0.0149 (6)
C3	0.04486 (16)	0.63610 (15)	0.2559 (5)	0.0165 (6)
H1	0.0145	0.6159	0.3788	0.020*
C4	0.09205 (16)	0.70469 (15)	0.2614 (5)	0.0192 (6)
H2	0.0992	0.7383	0.3891	0.023*
C5	0.12706 (15)	0.71477 (15)	0.0434 (5)	0.0186 (6)
H3	0.1617	0.7562	0.0006	0.022*
C6	0.10137 (15)	0.65216 (15)	−0.0999 (5)	0.0172 (6)
H4	0.1153	0.6448	−0.2553	0.021*
C7	−0.10232 (17)	0.71039 (17)	−0.1308 (6)	0.0285 (7)
H5	−0.1283	0.6643	−0.1836	0.034*
C8	−0.10795 (16)	0.74232 (16)	0.0892 (5)	0.0245 (7)
H6	−0.1383	0.7215	0.2111	0.029*
C9	−0.06075 (16)	0.81070 (16)	0.0981 (5)	0.0223 (6)
H7	−0.0540	0.8440	0.2268	0.027*

C10	−0.02530 (16)	0.82111 (16)	−0.1169 (5)	0.0230 (7)
H8	0.0096	0.8624	−0.1586	0.028*
C11	−0.05117 (18)	0.75871 (18)	−0.2605 (5)	0.0271 (7)
H9	−0.0367	0.7509	−0.4153	0.032*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0127 (2)	0.0098 (2)	0.0177 (2)	0.00023 (15)	−0.00097 (16)	0.00126 (15)
F1	0.0289 (9)	0.0176 (8)	0.0136 (8)	−0.0035 (7)	0.0007 (7)	0.0001 (6)
C1	0.0166 (13)	0.0157 (13)	0.0125 (14)	0.0038 (10)	−0.0015 (11)	−0.0008 (10)
C2	0.0145 (13)	0.0111 (12)	0.0191 (15)	0.0038 (10)	−0.0028 (11)	0.0015 (11)
C3	0.0210 (14)	0.0133 (13)	0.0152 (14)	0.0036 (11)	−0.0022 (11)	0.0017 (11)
C4	0.0219 (15)	0.0151 (14)	0.0204 (15)	0.0039 (11)	−0.0082 (12)	−0.0015 (11)
C5	0.0117 (13)	0.0139 (13)	0.0303 (17)	0.0010 (11)	−0.0020 (11)	0.0021 (12)
C6	0.0141 (13)	0.0158 (14)	0.0218 (15)	0.0035 (11)	0.0016 (11)	0.0011 (12)
C7	0.0192 (15)	0.0178 (15)	0.048 (2)	0.0014 (12)	−0.0167 (14)	−0.0025 (14)
C8	0.0149 (14)	0.0209 (15)	0.0378 (18)	0.0041 (12)	0.0040 (13)	0.0062 (13)
C9	0.0217 (15)	0.0146 (14)	0.0307 (16)	0.0075 (11)	−0.0019 (13)	−0.0024 (12)
C10	0.0186 (15)	0.0137 (14)	0.0368 (18)	0.0038 (11)	−0.0012 (13)	0.0111 (13)
C11	0.0284 (16)	0.0330 (17)	0.0198 (16)	0.0163 (14)	−0.0064 (13)	0.0023 (13)

Geometric parameters (Å, °)

Fe1—C3	2.041 (3)	C3—H1	0.9500
Fe1—C6	2.042 (3)	C4—C5	1.420 (4)
Fe1—C11	2.042 (3)	C4—H2	0.9500
Fe1—C10	2.043 (3)	C5—C6	1.423 (4)
Fe1—C7	2.044 (3)	C5—H3	0.9500
Fe1—C4	2.046 (3)	C6—H4	0.9500
Fe1—C8	2.047 (3)	C7—C8	1.403 (4)
Fe1—C5	2.047 (3)	C7—C11	1.416 (4)
Fe1—C9	2.049 (3)	C7—H5	0.9500
Fe1—C2	2.050 (3)	C8—C9	1.411 (4)
F1—C1	1.365 (3)	C8—H6	0.9500
C1—C1^{i}	1.331 (5)	C9—C10	1.408 (4)
C1—C2	1.448 (4)	C9—H7	0.9500
C2—C6	1.432 (4)	C10—C11	1.422 (4)
C2—C3	1.439 (4)	C10—H8	0.9500
C3—C4	1.413 (4)	C11—H9	0.9500
C3—Fe1—C6	69.03 (11)	C4—C3—C2	108.0 (2)
C3—Fe1—C11	159.96 (12)	C4—C3—Fe1	69.95 (15)
C6—Fe1—C11	107.59 (12)	C2—C3—Fe1	69.76 (14)
C3—Fe1—C10	157.77 (11)	C4—C3—H1	126.0
C6—Fe1—C10	122.70 (11)	C2—C3—H1	126.0
C11—Fe1—C10	40.76 (12)	Fe1—C3—H1	125.9
C3—Fe1—C7	123.69 (12)	C3—C4—C5	108.4 (2)
C6—Fe1—C7	123.51 (12)	C3—C4—Fe1	69.59 (15)

C11—Fe1—C7	40.55 (12)	C5—C4—Fe1	69.75 (15)
C10—Fe1—C7	68.15 (11)	C3—C4—H2	125.8
C3—Fe1—C4	40.46 (11)	C5—C4—H2	125.8
C6—Fe1—C4	68.65 (11)	Fe1—C4—H2	126.4
C11—Fe1—C4	158.40 (12)	C4—C5—C6	108.3 (2)
C10—Fe1—C4	122.05 (11)	C4—C5—Fe1	69.63 (15)
C7—Fe1—C4	159.15 (13)	C6—C5—Fe1	69.42 (15)
C3—Fe1—C8	107.93 (11)	C4—C5—H3	125.9
C6—Fe1—C8	159.45 (11)	C6—C5—H3	125.9
C11—Fe1—C8	67.89 (12)	Fe1—C5—H3	126.7
C10—Fe1—C8	67.89 (11)	C5—C6—C2	107.8 (2)
C7—Fe1—C8	40.10 (13)	C5—C6—Fe1	69.85 (15)
C4—Fe1—C8	123.07 (12)	C2—C6—Fe1	69.85 (14)
C3—Fe1—C5	68.41 (11)	C5—C6—H4	126.1
C6—Fe1—C5	40.73 (11)	C2—C6—H4	126.1
C11—Fe1—C5	122.74 (12)	Fe1—C6—H4	125.8
C10—Fe1—C5	107.10 (11)	C8—C7—C11	108.2 (3)
C7—Fe1—C5	159.27 (13)	C8—C7—Fe1	70.06 (17)
C4—Fe1—C5	40.61 (11)	C11—C7—Fe1	69.62 (16)
C8—Fe1—C5	158.73 (12)	C8—C7—H5	125.9
C3—Fe1—C9	122.43 (11)	C11—C7—H5	125.9
C6—Fe1—C9	158.57 (11)	Fe1—C7—H5	126.0
C11—Fe1—C9	67.98 (12)	C7—C8—C9	108.2 (3)
C10—Fe1—C9	40.27 (12)	C7—C8—Fe1	69.84 (16)
C7—Fe1—C9	67.69 (12)	C9—C8—Fe1	69.91 (16)
C4—Fe1—C9	107.31 (11)	C7—C8—H6	125.9
C8—Fe1—C9	40.30 (11)	C9—C8—H6	125.9
C5—Fe1—C9	122.60 (11)	Fe1—C8—H6	125.9
C3—Fe1—C2	41.17 (10)	C10—C9—C8	108.2 (3)
C6—Fe1—C2	40.96 (10)	C10—C9—Fe1	69.64 (15)
C11—Fe1—C2	123.42 (11)	C8—C9—Fe1	69.79 (16)
C10—Fe1—C2	159.43 (12)	C10—C9—H7	125.9
C7—Fe1—C2	108.40 (11)	C8—C9—H7	125.9
C4—Fe1—C2	68.58 (10)	Fe1—C9—H7	126.2
C8—Fe1—C2	123.44 (11)	C9—C10—C11	107.8 (3)
C5—Fe1—C2	68.53 (10)	C9—C10—Fe1	70.09 (15)
C9—Fe1—C2	159.04 (11)	C11—C10—Fe1	69.57 (16)
$C1^{i}$—C1—F1	116.2 (3)	C9—C10—H8	126.1
$C1^{i}$—C1—C2	130.4 (3)	C11—C10—H8	126.1
F1—C1—C2	113.4 (2)	Fe1—C10—H8	125.8
C6—C2—C3	107.4 (2)	C7—C11—C10	107.6 (3)
C6—C2—C1	123.7 (2)	C7—C11—Fe1	69.83 (16)
C3—C2—C1	128.8 (2)	C10—C11—Fe1	69.67 (16)
C6—C2—Fe1	69.20 (14)	C7—C11—H9	126.2
C3—C2—Fe1	69.06 (14)	C10—C11—H9	126.2
C1—C2—Fe1	127.83 (18)	Fe1—C11—H9	125.9
$C1^{i}$—C1—C2—C6	161.0 (3)	C2—Fe1—C6—C5	−118.8 (2)
F1—C1—C2—C6	−16.4 (4)	C3—Fe1—C6—C2	37.98 (15)

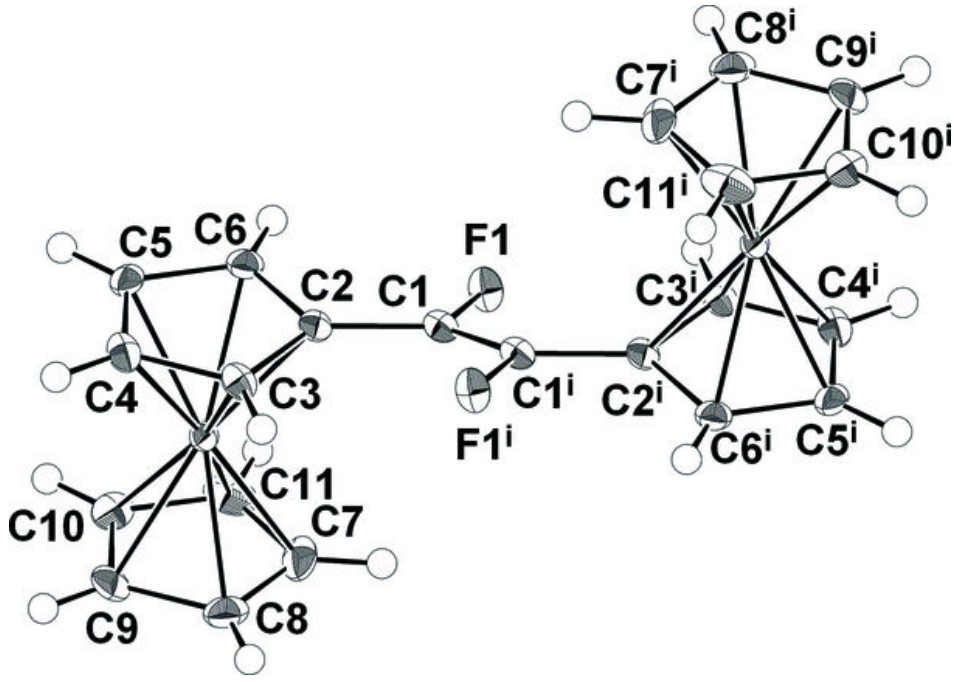
$C1^{i}$—C1—C2—C3	−17.7 (6)	C11—Fe1—C6—C2	−121.08 (17)
F1—C1—C2—C3	164.9 (2)	C10—Fe1—C6—C2	−163.28 (16)
$C1^{i}$—C1—C2—Fe1	−110.3 (4)	C7—Fe1—C6—C2	−79.33 (19)
F1—C1—C2—Fe1	72.3 (3)	C4—Fe1—C6—C2	81.50 (17)
C3—Fe1—C2—C6	−119.2 (2)	C8—Fe1—C6—C2	−47.3 (4)
C11—Fe1—C2—C6	78.00 (19)	C5—Fe1—C6—C2	118.8 (2)
C10—Fe1—C2—C6	43.6 (4)	C9—Fe1—C6—C2	164.5 (3)
C7—Fe1—C2—C6	120.28 (18)	C3—Fe1—C7—C8	77.46 (19)
C4—Fe1—C2—C6	−81.68 (17)	C6—Fe1—C7—C8	163.19 (16)
C8—Fe1—C2—C6	162.00 (17)	C11—Fe1—C7—C8	−119.3 (2)
C5—Fe1—C2—C6	−37.89 (16)	C10—Fe1—C7—C8	−81.18 (18)
C9—Fe1—C2—C6	−164.2 (3)	C4—Fe1—C7—C8	42.4 (4)
C6—Fe1—C2—C3	119.2 (2)	C5—Fe1—C7—C8	−161.7 (3)
C11—Fe1—C2—C3	−162.78 (17)	C9—Fe1—C7—C8	−37.57 (16)
C10—Fe1—C2—C3	162.8 (3)	C2—Fe1—C7—C8	120.43 (17)
C7—Fe1—C2—C3	−120.50 (17)	C3—Fe1—C7—C11	−163.24 (16)
C4—Fe1—C2—C3	37.54 (16)	C6—Fe1—C7—C11	−77.5 (2)
C8—Fe1—C2—C3	−78.78 (19)	C10—Fe1—C7—C11	38.12 (17)
C5—Fe1—C2—C3	81.32 (17)	C4—Fe1—C7—C11	161.7 (3)
C9—Fe1—C2—C3	−45.0 (4)	C8—Fe1—C7—C11	119.3 (2)
C3—Fe1—C2—C1	123.6 (3)	C5—Fe1—C7—C11	−42.4 (4)
C6—Fe1—C2—C1	−117.2 (3)	C9—Fe1—C7—C11	81.73 (18)
C11—Fe1—C2—C1	−39.2 (3)	C2—Fe1—C7—C11	−120.27 (17)
C10—Fe1—C2—C1	−73.6 (4)	C11—C7—C8—C9	0.2 (3)
C7—Fe1—C2—C1	3.1 (3)	Fe1—C7—C8—C9	59.59 (19)
C4—Fe1—C2—C1	161.1 (3)	C11—C7—C8—Fe1	−59.38 (19)
C8—Fe1—C2—C1	44.8 (3)	C3—Fe1—C8—C7	−121.39 (17)
C5—Fe1—C2—C1	−155.1 (3)	C6—Fe1—C8—C7	−43.4 (4)
C9—Fe1—C2—C1	78.6 (4)	C11—Fe1—C8—C7	37.73 (18)
C6—C2—C3—C4	−0.9 (3)	C10—Fe1—C8—C7	81.88 (19)
C1—C2—C3—C4	177.9 (3)	C4—Fe1—C8—C7	−163.35 (17)
Fe1—C2—C3—C4	−59.72 (18)	C5—Fe1—C8—C7	162.2 (3)
C6—C2—C3—Fe1	58.77 (17)	C9—Fe1—C8—C7	119.3 (3)
C1—C2—C3—Fe1	−122.3 (3)	C2—Fe1—C8—C7	−78.6 (2)
C6—Fe1—C3—C4	81.28 (17)	C3—Fe1—C8—C9	119.33 (18)
C11—Fe1—C3—C4	165.2 (3)	C6—Fe1—C8—C9	−162.7 (3)
C10—Fe1—C3—C4	−45.0 (4)	C11—Fe1—C8—C9	−81.56 (19)
C7—Fe1—C3—C4	−161.65 (17)	C10—Fe1—C8—C9	−37.41 (18)
C8—Fe1—C3—C4	−120.29 (17)	C7—Fe1—C8—C9	−119.3 (3)
C5—Fe1—C3—C4	37.42 (16)	C4—Fe1—C8—C9	77.4 (2)
C9—Fe1—C3—C4	−78.37 (19)	C5—Fe1—C8—C9	42.9 (4)
C2—Fe1—C3—C4	119.1 (2)	C2—Fe1—C8—C9	162.07 (17)
C6—Fe1—C3—C2	−37.78 (15)	C7—C8—C9—C10	−0.3 (3)
C11—Fe1—C3—C2	46.1 (4)	Fe1—C8—C9—C10	59.25 (19)
C10—Fe1—C3—C2	−164.1 (3)	C7—C8—C9—Fe1	−59.55 (19)
C7—Fe1—C3—C2	79.28 (19)	C3—Fe1—C9—C10	161.21 (16)
C4—Fe1—C3—C2	−119.1 (2)	C6—Fe1—C9—C10	43.9 (4)
C8—Fe1—C3—C2	120.65 (16)	C11—Fe1—C9—C10	−38.12 (18)

C5—Fe1—C3—C2	−81.64 (16)	C7—Fe1—C9—C10	−82.06 (19)
C9—Fe1—C3—C2	162.57 (15)	C4—Fe1—C9—C10	119.47 (17)
C2—C3—C4—C5	0.5 (3)	C8—Fe1—C9—C10	−119.5 (3)
Fe1—C3—C4—C5	−59.14 (18)	C5—Fe1—C9—C10	77.6 (2)
C2—C3—C4—Fe1	59.60 (18)	C2—Fe1—C9—C10	−165.3 (3)
C6—Fe1—C4—C3	−82.31 (16)	C3—Fe1—C9—C8	−79.3 (2)
C11—Fe1—C4—C3	−166.2 (3)	C6—Fe1—C9—C8	163.4 (3)
C10—Fe1—C4—C3	161.61 (16)	C11—Fe1—C9—C8	81.3 (2)
C7—Fe1—C4—C3	47.4 (4)	C10—Fe1—C9—C8	119.5 (3)
C8—Fe1—C4—C3	78.63 (19)	C7—Fe1—C9—C8	37.39 (18)
C5—Fe1—C4—C3	−119.8 (2)	C4—Fe1—C9—C8	−121.07 (18)
C9—Fe1—C4—C3	120.01 (16)	C5—Fe1—C9—C8	−162.96 (17)
C2—Fe1—C4—C3	−38.18 (16)	C2—Fe1—C9—C8	−45.9 (4)
C3—Fe1—C4—C5	119.8 (2)	C8—C9—C10—C11	0.3 (3)
C6—Fe1—C4—C5	37.44 (16)	Fe1—C9—C10—C11	59.61 (18)
C11—Fe1—C4—C5	−46.5 (4)	C8—C9—C10—Fe1	−59.34 (19)
C10—Fe1—C4—C5	−78.64 (19)	C3—Fe1—C10—C9	−45.9 (4)
C7—Fe1—C4—C5	167.2 (3)	C6—Fe1—C10—C9	−162.47 (16)
C8—Fe1—C4—C5	−161.61 (16)	C11—Fe1—C10—C9	118.8 (2)
C9—Fe1—C4—C5	−120.23 (16)	C7—Fe1—C10—C9	80.83 (19)
C2—Fe1—C4—C5	81.58 (17)	C4—Fe1—C10—C9	−78.70 (19)
C3—C4—C5—C6	0.2 (3)	C8—Fe1—C10—C9	37.44 (17)
Fe1—C4—C5—C6	−58.83 (18)	C5—Fe1—C10—C9	−120.59 (17)
C3—C4—C5—Fe1	59.03 (18)	C2—Fe1—C10—C9	165.1 (3)
C3—Fe1—C5—C4	−37.29 (15)	C3—Fe1—C10—C11	−164.7 (3)
C6—Fe1—C5—C4	−119.8 (2)	C6—Fe1—C10—C11	78.8 (2)
C11—Fe1—C5—C4	161.50 (16)	C7—Fe1—C10—C11	−37.93 (18)
C10—Fe1—C5—C4	119.61 (17)	C4—Fe1—C10—C11	162.54 (17)
C7—Fe1—C5—C4	−167.1 (3)	C8—Fe1—C10—C11	−81.33 (19)
C8—Fe1—C5—C4	46.8 (4)	C5—Fe1—C10—C11	120.65 (18)
C9—Fe1—C5—C4	78.27 (19)	C9—Fe1—C10—C11	−118.8 (2)
C2—Fe1—C5—C4	−81.71 (17)	C2—Fe1—C10—C11	46.3 (4)
C3—Fe1—C5—C6	82.51 (17)	C8—C7—C11—C10	0.0 (3)
C11—Fe1—C5—C6	−78.70 (19)	Fe1—C7—C11—C10	−59.69 (19)
C10—Fe1—C5—C6	−120.59 (17)	C8—C7—C11—Fe1	59.7 (2)
C7—Fe1—C5—C6	−47.3 (4)	C9—C10—C11—C7	−0.1 (3)
C4—Fe1—C5—C6	119.8 (2)	Fe1—C10—C11—C7	59.79 (19)
C8—Fe1—C5—C6	166.6 (3)	C9—C10—C11—Fe1	−59.94 (18)
C9—Fe1—C5—C6	−161.93 (16)	C3—Fe1—C11—C7	44.4 (4)
C2—Fe1—C5—C6	38.09 (16)	C6—Fe1—C11—C7	121.34 (17)
C4—C5—C6—C2	−0.8 (3)	C10—Fe1—C11—C7	−118.6 (2)
Fe1—C5—C6—C2	−59.76 (17)	C4—Fe1—C11—C7	−162.4 (3)
C4—C5—C6—Fe1	58.96 (18)	C8—Fe1—C11—C7	−37.32 (17)
C3—C2—C6—C5	1.1 (3)	C5—Fe1—C11—C7	163.51 (17)
C1—C2—C6—C5	−177.9 (2)	C9—Fe1—C11—C7	−80.96 (18)
Fe1—C2—C6—C5	59.76 (18)	C2—Fe1—C11—C7	79.1 (2)
C3—C2—C6—Fe1	−58.68 (17)	C3—Fe1—C11—C10	163.1 (3)
C1—C2—C6—Fe1	122.4 (2)	C6—Fe1—C11—C10	−120.02 (17)
C3—Fe1—C6—C5	−80.86 (17)	C7—Fe1—C11—C10	118.6 (2)

C11—Fe1—C6—C5	120.08 (17)	C4—Fe1—C11—C10	−43.7 (4)
C10—Fe1—C6—C5	77.88 (19)	C8—Fe1—C11—C10	81.32 (18)
C7—Fe1—C6—C5	161.83 (17)	C5—Fe1—C11—C10	−77.85 (19)
C4—Fe1—C6—C5	−37.34 (16)	C9—Fe1—C11—C10	37.67 (17)
C8—Fe1—C6—C5	−166.1 (3)	C2—Fe1—C11—C10	−162.29 (16)
C9—Fe1—C6—C5	45.7 (4)		

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

Fig. 1


C8i
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C7
C9
C8

Fig. 2