Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-[(2,3,4,5,6-Pentafluorophenyl)ethynyl]-ferrocene

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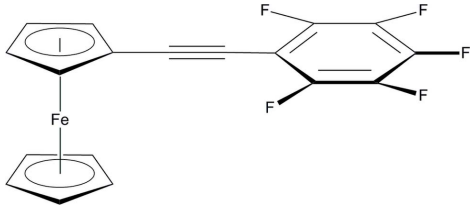
Received 29 June 2010; accepted 6 July 2010

Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.005 Å; R factor = 0.040; wR factor = 0.105; data-to-parameter ratio = 11.7.

The molecular structure of the title compound, [Fe(C_5H_5)($C_{13}H_4F_5$)], consists of a ferrocenyl group and a 2,3,4,5,6-pentafluorobenzene group linked through an ethyne spacer. The crystal packing is dominated by intermolecular C—H···F hydrogen bonds, C—F···π interactions between the pentafluorobenzene groups [F···centroid distances = 3.882 (2) and 3.884 (2) Å] and π–π interactions between the pentafluorobenzene and cyclopentadienyl rings [centroid–centroid distance = 3.741 (1) Å].

Related literature

For general background to ferrocene derivatives, see: Debroy & Roy (2007). For a related structure, see: Valdebenito *et al.* (2010). For the synthesis, see: Torres *et al.* (2002); Zora *et al.* (2006).



Experimental

Crystal data

[Fe(C_5H_5)($C_{13}H_4F_5$)]
M_r = 376.10
Triclinic, $P\overline{1}$
a = 6.0767 (9) Å
b = 10.7164 (15) Å
c = 12.6014 (18) Å
α = 65.725 (2)°
β = 89.364 (3)°
γ = 78.726 (2)°
V = 731.41 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.08 mm^{-1}
T = 292 K
0.30 × 0.04 × 0.02 mm

Data collection

Bruker SMART APEX CCD diffractometer
4793 measured reflections
2533 independent reflections
2169 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.105
S = 1.05
2533 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···F5^{i}	0.93	2.50	3.176 (3)	130

Symmetry code: (i) $-x+1, -y+2, -z+2$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to Mr Xianggao Meng for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2327).

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supporting information

Acta Cryst. (2010). E**66**, m914 [https://doi.org/10.1107/S1600536810026772]

1-[(2,3,4,5,6-Pentafluorophenyl)ethynyl]ferrocene

Chan Zhang, Honglin Zhang, Dongdong Dai and Jinhua Liang

S1. Comment

Ferrocene derivatives with linear, unsaturated side-arms show altered unique properties, such as electrical conductivity, thermal stability, magnetic, electronic, redox and non-linear optical behaviors, compared to their saturated derivatives (Debroy & Roy, 2007).

The molecular structure of the title compound is composed of a ferrocenyl group and a pentafluorobenzene group joined by an organic ethyne spacer. Two cyclopentadienyl rings of the ferrocenyl group are parallel (Valdebenito *et al.*, 2010). The main features of the structure are an intermolecular C—H···F hydrogen bond between the ferrocenyl and pentafluorobenzene (Table 1), C—F···π interactions between the pentafluorobenzene groups [F···centroid distances = 3.882 (2) and 3.884 (2) Å] and a π–π interaction between the pentafluorobenzene and cyclopentadienyl rings [centroid–centroid distance = 3.741 (1) Å].

S2. Experimental

The title compound was synthesized according to a modified literature procedure (Torres *et al.*, 2002; Zora *et al.*, 2006). 1,2,3,4,5-Pentafluoro-6-iodobenzene (735 mg, 2.5 mmol) and ethynylferrocene (525 mg, 2.5 mmol) were added to a mixture of $Cu(CH_3CO_2)_2$ (40 mg, 0.2 mmol), $Pd(PPh_3)_2Cl_2$ (140 mg, 0.2 mmol) and $^iPr_2NH$ (30 ml) under argon. The resulting mixture was refluxed at 365 K for 18 h. The solution was then extracted with dichloromethane, washed with water and dried over Na_2SO_4. Final purification was achieved by flash column chromatography on silica gel using dichloromethane/petroleum (1:4) as eluant. The product was obtained in 30% yield. Crystals of the title compound suitable for X-ray diffraction were obtained by slow evaporation of a solution of the compound in dichloromethane/hexane (1:10 v/v) at room temperature.

S3. Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

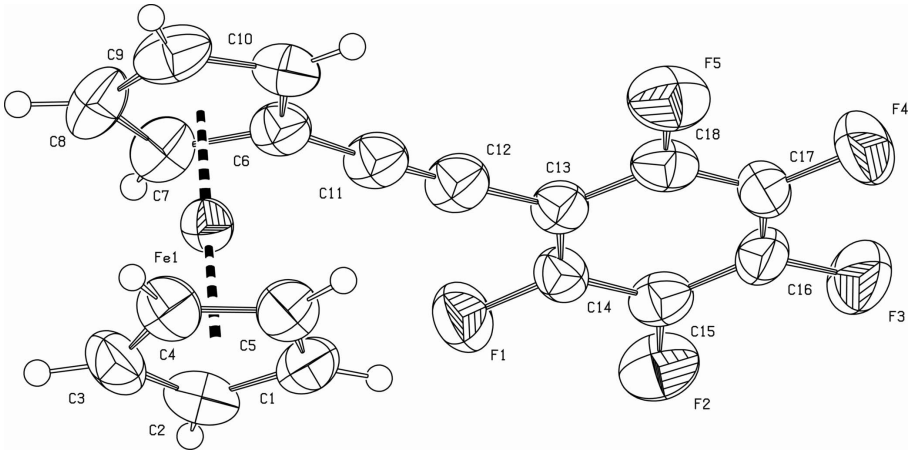

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

1-[(2,3,4,5,6-Pentafluorophenyl)ethynyl]ferrocene

Crystal data

$[Fe(C_5H_5)(C_{13}H_4F_5)]$
$M_r = 376.10$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.0767\ (9)$ Å
$b = 10.7164\ (15)$ Å
$c = 12.6014\ (18)$ Å
$\alpha = 65.725\ (2)°$
$\beta = 89.364\ (3)°$
$\gamma = 78.726\ (2)°$
$V = 731.41\ (18)$ Å^3
$Z = 2$
$F(000) = 376$
$D_x = 1.708$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1760 reflections
$\theta = 3.3–25.1°$
$\mu = 1.08$ mm^{-1}
$T = 292$ K
Plate, yellow
0.30 × 0.04 × 0.02 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
4793 measured reflections
2533 independent reflections
2169 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
$h = -7\rightarrow7$
$k = -12\rightarrow12$
$l = -13\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.105$
$S = 1.05$
2533 reflections
217 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.0784P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.72848 (6)	0.78028 (4)	0.74835 (3)	0.03952 (17)
C1	0.7513 (5)	0.5868 (3)	0.8801 (3)	0.0544 (8)
H1	0.7967	0.5607	0.9578	0.065*
C2	0.8930 (6)	0.5793 (3)	0.7932 (3)	0.0603 (9)
H2	1.0483	0.5472	0.8031	0.072*
C3	0.7575 (6)	0.6290 (3)	0.6885 (3)	0.0629 (9)
H3	0.8079	0.6360	0.6167	0.075*
C4	0.5318 (5)	0.6666 (3)	0.7110 (3)	0.0550 (8)
H4	0.4074	0.7022	0.6570	0.066*
C5	0.5292 (5)	0.6405 (3)	0.8295 (3)	0.0534 (8)
H5	0.4024	0.6561	0.8679	0.064*
C6	0.8628 (5)	0.8977 (3)	0.8131 (3)	0.0466 (7)
C7	0.9602 (5)	0.9037 (3)	0.7080 (3)	0.0537 (8)
H7	1.1120	0.8756	0.7001	0.064*
C8	0.7850 (6)	0.9598 (3)	0.6182 (3)	0.0612 (9)
H8	0.8017	0.9753	0.5406	0.073*
C9	0.5823 (6)	0.9883 (3)	0.6656 (3)	0.0620 (9)
H9	0.4417	1.0264	0.6245	0.074*
C10	0.6256 (5)	0.9498 (3)	0.7858 (3)	0.0535 (8)
H10	0.5195	0.9569	0.8379	0.064*
C11	0.9780 (5)	0.8492 (3)	0.9247 (3)	0.0506 (7)
C12	1.0717 (5)	0.8129 (3)	1.0184 (3)	0.0524 (7)
C13	1.1670 (5)	0.7703 (3)	1.1340 (2)	0.0434 (6)
C14	1.3917 (5)	0.7049 (3)	1.1689 (2)	0.0441 (7)
C15	1.4796 (5)	0.6621 (3)	1.2811 (3)	0.0496 (7)
C16	1.3452 (6)	0.6841 (3)	1.3614 (2)	0.0539 (8)
C17	1.1218 (6)	0.7482 (3)	1.3302 (3)	0.0551 (8)
C18	1.0362 (5)	0.7906 (3)	1.2187 (3)	0.0518 (8)
F1	1.5272 (3)	0.68281 (19)	1.09132 (16)	0.0650 (5)
F2	1.6961 (3)	0.59629 (19)	1.31194 (17)	0.0709 (5)
F3	1.4306 (4)	0.6459 (2)	1.46997 (16)	0.0892 (7)
F4	0.9884 (4)	0.7688 (2)	1.40989 (18)	0.0896 (7)
F5	0.8196 (3)	0.85479 (19)	1.19000 (19)	0.0741 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0398 (3)	0.0418 (3)	0.0403 (3)	−0.01159 (17)	0.00257 (18)	−0.01908 (19)
C1	0.067 (2)	0.0416 (15)	0.0485 (18)	−0.0124 (14)	−0.0050 (16)	−0.0118 (14)
C2	0.0542 (19)	0.0474 (17)	0.085 (3)	−0.0053 (14)	0.0022 (18)	−0.0358 (17)
C3	0.085 (2)	0.0606 (19)	0.065 (2)	−0.0260 (17)	0.0217 (19)	−0.0425 (18)
C4	0.0571 (19)	0.0602 (18)	0.060 (2)	−0.0209 (15)	−0.0019 (16)	−0.0336 (16)
C5	0.0535 (19)	0.0519 (17)	0.059 (2)	−0.0222 (14)	0.0127 (16)	−0.0228 (15)
C6	0.0520 (18)	0.0408 (14)	0.0502 (17)	−0.0126 (12)	−0.0047 (14)	−0.0207 (13)
C7	0.0466 (17)	0.0569 (17)	0.057 (2)	−0.0210 (14)	0.0025 (15)	−0.0188 (15)

C8	0.069 (2)	0.0617 (19)	0.0443 (18)	−0.0308 (17)	−0.0013 (16)	−0.0060 (15)
C9	0.056 (2)	0.0463 (17)	0.071 (2)	−0.0078 (14)	−0.0208 (17)	−0.0127 (16)
C10	0.0512 (18)	0.0439 (15)	0.067 (2)	−0.0031 (13)	−0.0014 (15)	−0.0278 (15)
C11	0.0554 (19)	0.0433 (15)	0.0563 (19)	−0.0155 (13)	−0.0044 (15)	−0.0215 (14)
C12	0.0585 (19)	0.0470 (16)	0.055 (2)	−0.0173 (14)	−0.0031 (16)	−0.0210 (15)
C13	0.0499 (17)	0.0384 (14)	0.0460 (16)	−0.0157 (12)	0.0008 (13)	−0.0188 (13)
C14	0.0471 (17)	0.0444 (14)	0.0464 (17)	−0.0138 (12)	0.0086 (14)	−0.0228 (13)
C15	0.0514 (18)	0.0406 (15)	0.0554 (19)	−0.0124 (13)	−0.0034 (15)	−0.0173 (14)
C16	0.085 (2)	0.0417 (15)	0.0356 (16)	−0.0192 (15)	−0.0014 (16)	−0.0136 (13)
C17	0.080 (2)	0.0444 (16)	0.0496 (19)	−0.0222 (15)	0.0240 (17)	−0.0240 (14)
C18	0.0484 (18)	0.0395 (15)	0.068 (2)	−0.0123 (13)	0.0092 (16)	−0.0218 (15)
F1	0.0653 (12)	0.0744 (11)	0.0630 (11)	−0.0143 (9)	0.0201 (9)	−0.0366 (10)
F2	0.0557 (12)	0.0658 (11)	0.0808 (13)	−0.0075 (9)	−0.0152 (10)	−0.0222 (10)
F3	0.147 (2)	0.0710 (12)	0.0463 (11)	−0.0216 (13)	−0.0146 (12)	−0.0211 (10)
F4	0.1264 (19)	0.0795 (13)	0.0750 (13)	−0.0281 (12)	0.0557 (13)	−0.0424 (11)
F5	0.0497 (11)	0.0640 (11)	0.1014 (15)	−0.0069 (9)	0.0147 (10)	−0.0299 (11)

Geometric parameters (Å, º)

Fe1—C3	2.029 (3)	C6—C10	1.430 (4)
Fe1—C2	2.032 (3)	C7—C8	1.411 (4)
Fe1—C1	2.034 (3)	C7—H7	0.9300
Fe1—C7	2.037 (3)	C8—C9	1.398 (4)
Fe1—C8	2.040 (3)	C8—H8	0.9300
Fe1—C10	2.042 (3)	C9—C10	1.409 (4)
Fe1—C5	2.044 (3)	C9—H9	0.9300
Fe1—C6	2.044 (3)	C10—H10	0.9300
Fe1—C9	2.045 (3)	C11—C12	1.191 (4)
Fe1—C4	2.047 (3)	C12—C13	1.427 (4)
C1—C2	1.404 (4)	C13—C18	1.386 (4)
C1—C5	1.405 (4)	C13—C14	1.391 (4)
C1—H1	0.9300	C14—F1	1.336 (3)
C2—C3	1.406 (5)	C14—C15	1.372 (4)
C2—H2	0.9300	C15—F2	1.342 (3)
C3—C4	1.412 (4)	C15—C16	1.360 (4)
C3—H3	0.9300	C16—F3	1.335 (3)
C4—C5	1.402 (4)	C16—C17	1.376 (5)
C4—H4	0.9300	C17—F4	1.345 (3)
C5—H5	0.9300	C17—C18	1.360 (4)
C6—C11	1.421 (4)	C18—F5	1.337 (3)
C6—C7	1.426 (4)		
C3—Fe1—C2	40.51 (13)	C5—C4—C3	107.6 (3)
C3—Fe1—C1	67.85 (13)	C5—C4—Fe1	69.83 (16)
C2—Fe1—C1	40.41 (12)	C3—C4—Fe1	69.08 (17)
C3—Fe1—C7	118.88 (13)	C5—C4—H4	126.2
C2—Fe1—C7	108.34 (13)	C3—C4—H4	126.2
C1—Fe1—C7	128.23 (13)	Fe1—C4—H4	126.4

C3—Fe1—C8	109.38 (14)	C4—C5—C1	108.2 (3)
C2—Fe1—C8	129.09 (14)	C4—C5—Fe1	70.07 (16)
C1—Fe1—C8	166.63 (13)	C1—C5—Fe1	69.47 (16)
C7—Fe1—C8	40.51 (12)	C4—C5—H5	125.9
C3—Fe1—C10	166.11 (14)	C1—C5—H5	125.9
C2—Fe1—C10	151.56 (14)	Fe1—C5—H5	126.1
C1—Fe1—C10	117.85 (13)	C11—C6—C7	126.8 (3)
C7—Fe1—C10	68.73 (12)	C11—C6—C10	125.8 (3)
C8—Fe1—C10	68.07 (14)	C7—C6—C10	107.4 (3)
C3—Fe1—C5	67.75 (13)	C11—C6—Fe1	126.48 (19)
C2—Fe1—C5	67.92 (13)	C7—C6—Fe1	69.29 (15)
C1—Fe1—C5	40.30 (12)	C10—C6—Fe1	69.44 (16)
C7—Fe1—C5	165.96 (12)	C8—C7—C6	107.7 (3)
C8—Fe1—C5	152.15 (13)	C8—C7—Fe1	69.85 (17)
C10—Fe1—C5	107.70 (13)	C6—C7—Fe1	69.79 (16)
C3—Fe1—C6	152.12 (14)	C8—C7—H7	126.1
C2—Fe1—C6	117.98 (13)	C6—C7—H7	126.1
C1—Fe1—C6	107.64 (12)	Fe1—C7—H7	125.8
C7—Fe1—C6	40.92 (11)	C9—C8—C7	108.5 (3)
C8—Fe1—C6	68.29 (13)	C9—C8—Fe1	70.17 (17)
C10—Fe1—C6	40.98 (11)	C7—C8—Fe1	69.64 (17)
C5—Fe1—C6	127.66 (12)	C9—C8—H8	125.8
C3—Fe1—C9	129.10 (14)	C7—C8—H8	125.8
C2—Fe1—C9	166.84 (14)	Fe1—C8—H8	126.0
C1—Fe1—C9	151.75 (14)	C8—C9—C10	108.9 (3)
C7—Fe1—C9	67.90 (13)	C8—C9—Fe1	69.80 (18)
C8—Fe1—C9	40.03 (13)	C10—C9—Fe1	69.72 (16)
C10—Fe1—C9	40.35 (12)	C8—C9—H9	125.5
C5—Fe1—C9	118.81 (13)	C10—C9—H9	125.5
C6—Fe1—C9	68.10 (12)	Fe1—C9—H9	126.5
C3—Fe1—C4	40.53 (13)	C9—C10—C6	107.4 (3)
C2—Fe1—C4	68.12 (13)	C9—C10—Fe1	69.93 (17)
C1—Fe1—C4	67.74 (13)	C6—C10—Fe1	69.58 (15)
C7—Fe1—C4	152.61 (13)	C9—C10—H10	126.3
C8—Fe1—C4	119.34 (13)	C6—C10—H10	126.3
C10—Fe1—C4	127.70 (12)	Fe1—C10—H10	125.8
C5—Fe1—C4	40.10 (12)	C12—C11—C6	177.7 (3)
C6—Fe1—C4	165.50 (12)	C11—C12—C13	175.5 (3)
C9—Fe1—C4	109.02 (13)	C18—C13—C14	116.4 (3)
C2—C1—C5	108.3 (3)	C18—C13—C12	120.9 (3)
C2—C1—Fe1	69.73 (17)	C14—C13—C12	122.7 (3)
C5—C1—Fe1	70.23 (16)	F1—C14—C15	118.6 (3)
C2—C1—H1	125.8	F1—C14—C13	119.4 (3)
C5—C1—H1	125.8	C15—C14—C13	122.0 (3)
Fe1—C1—H1	125.8	F2—C15—C16	120.2 (3)
C1—C2—C3	107.6 (3)	F2—C15—C14	120.1 (3)
C1—C2—Fe1	69.86 (16)	C16—C15—C14	119.6 (3)
C3—C2—Fe1	69.65 (17)	F3—C16—C15	120.0 (3)

C1—C2—H2	126.2	F3—C16—C17	119.9 (3)
C3—C2—H2	126.2	C15—C16—C17	120.0 (3)
Fe1—C2—H2	125.9	F4—C17—C18	120.1 (3)
C2—C3—C4	108.3 (3)	F4—C17—C16	120.0 (3)
C2—C3—Fe1	69.84 (17)	C18—C17—C16	119.9 (3)
C4—C3—Fe1	70.39 (17)	F5—C18—C17	118.8 (3)
C2—C3—H3	125.8	F5—C18—C13	119.2 (3)
C4—C3—H3	125.8	C17—C18—C13	122.0 (3)
Fe1—C3—H3	125.5		

C3—Fe1—C1—C2	37.99 (19)	C1—Fe1—C6—C10	−112.43 (19)
C7—Fe1—C1—C2	−72.1 (2)	C7—Fe1—C6—C10	118.9 (3)
C8—Fe1—C1—C2	−42.6 (6)	C8—Fe1—C6—C10	81.1 (2)
C10—Fe1—C1—C2	−155.99 (19)	C5—Fe1—C6—C10	−72.4 (2)
C5—Fe1—C1—C2	119.2 (3)	C9—Fe1—C6—C10	37.84 (18)
C6—Fe1—C1—C2	−112.7 (2)	C4—Fe1—C6—C10	−43.4 (5)
C9—Fe1—C1—C2	170.9 (2)	C11—C6—C7—C8	−179.5 (3)
C4—Fe1—C1—C2	81.9 (2)	C10—C6—C7—C8	0.6 (3)
C3—Fe1—C1—C5	−81.3 (2)	Fe1—C6—C7—C8	59.8 (2)
C2—Fe1—C1—C5	−119.2 (3)	C11—C6—C7—Fe1	120.7 (3)
C7—Fe1—C1—C5	168.67 (17)	C10—C6—C7—Fe1	−59.20 (19)
C8—Fe1—C1—C5	−161.9 (5)	C3—Fe1—C7—C8	86.4 (2)
C10—Fe1—C1—C5	84.8 (2)	C2—Fe1—C7—C8	129.4 (2)
C6—Fe1—C1—C5	128.05 (18)	C1—Fe1—C7—C8	169.92 (19)
C9—Fe1—C1—C5	51.7 (3)	C10—Fe1—C7—C8	−80.7 (2)
C4—Fe1—C1—C5	−37.32 (18)	C5—Fe1—C7—C8	−158.5 (4)
C5—C1—C2—C3	0.2 (3)	C6—Fe1—C7—C8	−118.8 (3)
Fe1—C1—C2—C3	−59.7 (2)	C9—Fe1—C7—C8	−37.2 (2)
C5—C1—C2—Fe1	59.9 (2)	C4—Fe1—C7—C8	51.7 (4)
C3—Fe1—C2—C1	−118.6 (3)	C3—Fe1—C7—C6	−154.81 (18)
C7—Fe1—C2—C1	128.06 (19)	C2—Fe1—C7—C6	−111.85 (19)
C8—Fe1—C2—C1	168.36 (18)	C1—Fe1—C7—C6	−71.3 (2)
C10—Fe1—C2—C1	49.0 (3)	C8—Fe1—C7—C6	118.8 (3)
C5—Fe1—C2—C1	−37.52 (18)	C10—Fe1—C7—C6	38.03 (17)
C6—Fe1—C2—C1	84.6 (2)	C5—Fe1—C7—C6	−39.7 (6)
C9—Fe1—C2—C1	−160.8 (5)	C9—Fe1—C7—C6	81.60 (19)
C4—Fe1—C2—C1	−80.9 (2)	C4—Fe1—C7—C6	170.5 (2)
C1—Fe1—C2—C3	118.6 (3)	C6—C7—C8—C9	−0.1 (3)
C7—Fe1—C2—C3	−113.3 (2)	Fe1—C7—C8—C9	59.6 (2)
C8—Fe1—C2—C3	−73.0 (2)	C6—C7—C8—Fe1	−59.75 (19)
C10—Fe1—C2—C3	167.7 (2)	C3—Fe1—C8—C9	128.4 (2)
C5—Fe1—C2—C3	81.1 (2)	C2—Fe1—C8—C9	169.54 (19)
C6—Fe1—C2—C3	−156.79 (19)	C1—Fe1—C8—C9	−156.0 (5)
C9—Fe1—C2—C3	−42.2 (6)	C7—Fe1—C8—C9	−119.5 (3)
C4—Fe1—C2—C3	37.74 (18)	C10—Fe1—C8—C9	−37.05 (19)
C1—C2—C3—C4	−0.3 (3)	C5—Fe1—C8—C9	49.5 (4)
Fe1—C2—C3—C4	−60.1 (2)	C6—Fe1—C8—C9	−81.4 (2)
C1—C2—C3—Fe1	59.8 (2)	C4—Fe1—C8—C9	85.0 (2)

C1—Fe1—C3—C2	−37.89 (19)	C3—Fe1—C8—C7	−112.1 (2)
C7—Fe1—C3—C2	84.7 (2)	C2—Fe1—C8—C7	−70.9 (2)
C8—Fe1—C3—C2	128.1 (2)	C1—Fe1—C8—C7	−36.5 (6)
C10—Fe1—C3—C2	−155.0 (5)	C10—Fe1—C8—C7	82.5 (2)
C5—Fe1—C3—C2	−81.6 (2)	C5—Fe1—C8—C7	169.0 (2)
C6—Fe1—C3—C2	48.1 (3)	C6—Fe1—C8—C7	38.17 (19)
C9—Fe1—C3—C2	168.64 (19)	C9—Fe1—C8—C7	119.5 (3)
C4—Fe1—C3—C2	−119.1 (3)	C4—Fe1—C8—C7	−155.52 (19)
C2—Fe1—C3—C4	119.1 (3)	C7—C8—C9—C10	−0.4 (4)
C1—Fe1—C3—C4	81.2 (2)	Fe1—C8—C9—C10	58.9 (2)
C7—Fe1—C3—C4	−156.23 (18)	C7—C8—C9—Fe1	−59.3 (2)
C8—Fe1—C3—C4	−112.8 (2)	C3—Fe1—C9—C8	−72.4 (2)
C10—Fe1—C3—C4	−35.9 (6)	C2—Fe1—C9—C8	−38.2 (6)
C5—Fe1—C3—C4	37.50 (18)	C1—Fe1—C9—C8	168.5 (2)
C6—Fe1—C3—C4	167.2 (2)	C7—Fe1—C9—C8	37.59 (19)
C9—Fe1—C3—C4	−72.3 (2)	C10—Fe1—C9—C8	120.3 (3)
C2—C3—C4—C5	0.3 (3)	C5—Fe1—C9—C8	−156.08 (19)
Fe1—C3—C4—C5	−59.5 (2)	C6—Fe1—C9—C8	81.9 (2)
C2—C3—C4—Fe1	59.8 (2)	C4—Fe1—C9—C8	−113.3 (2)
C3—Fe1—C4—C5	119.0 (3)	C3—Fe1—C9—C10	167.30 (18)
C2—Fe1—C4—C5	81.3 (2)	C2—Fe1—C9—C10	−158.5 (5)
C1—Fe1—C4—C5	37.50 (18)	C1—Fe1—C9—C10	48.2 (3)
C7—Fe1—C4—C5	169.1 (2)	C7—Fe1—C9—C10	−82.72 (19)
C8—Fe1—C4—C5	−155.12 (19)	C8—Fe1—C9—C10	−120.3 (3)
C10—Fe1—C4—C5	−71.3 (2)	C5—Fe1—C9—C10	83.6 (2)
C6—Fe1—C4—C5	−36.5 (5)	C6—Fe1—C9—C10	−38.43 (18)
C9—Fe1—C4—C5	−112.5 (2)	C4—Fe1—C9—C10	126.40 (19)
C2—Fe1—C4—C3	−37.72 (19)	C8—C9—C10—C6	0.8 (3)
C1—Fe1—C4—C3	−81.5 (2)	Fe1—C9—C10—C6	59.73 (19)
C7—Fe1—C4—C3	50.1 (4)	C8—C9—C10—Fe1	−58.9 (2)
C8—Fe1—C4—C3	85.9 (2)	C11—C6—C10—C9	179.2 (3)
C10—Fe1—C4—C3	169.76 (19)	C7—C6—C10—C9	−0.8 (3)
C5—Fe1—C4—C3	−119.0 (3)	Fe1—C6—C10—C9	−60.0 (2)
C6—Fe1—C4—C3	−155.5 (4)	C11—C6—C10—Fe1	−120.8 (3)
C9—Fe1—C4—C3	128.6 (2)	C7—C6—C10—Fe1	59.11 (19)
C3—C4—C5—C1	−0.2 (3)	C3—Fe1—C10—C9	−45.3 (6)
Fe1—C4—C5—C1	−59.2 (2)	C2—Fe1—C10—C9	169.9 (2)
C3—C4—C5—Fe1	59.0 (2)	C1—Fe1—C10—C9	−156.46 (19)
C2—C1—C5—C4	0.0 (3)	C7—Fe1—C10—C9	80.5 (2)
Fe1—C1—C5—C4	59.6 (2)	C8—Fe1—C10—C9	36.76 (19)
C2—C1—C5—Fe1	−59.6 (2)	C5—Fe1—C10—C9	−113.9 (2)
C3—Fe1—C5—C4	−37.89 (19)	C6—Fe1—C10—C9	118.5 (3)
C2—Fe1—C5—C4	−81.8 (2)	C4—Fe1—C10—C9	−74.1 (2)
C1—Fe1—C5—C4	−119.4 (3)	C3—Fe1—C10—C6	−163.8 (5)
C7—Fe1—C5—C4	−158.9 (5)	C2—Fe1—C10—C6	51.5 (3)
C8—Fe1—C5—C4	51.7 (3)	C1—Fe1—C10—C6	85.1 (2)
C10—Fe1—C5—C4	128.14 (19)	C7—Fe1—C10—C6	−37.97 (17)
C6—Fe1—C5—C4	169.15 (17)	C8—Fe1—C10—C6	−81.69 (19)

C9—Fe1—C5—C4	85.7 (2)	C5—Fe1—C10—C6	127.62 (18)
C3—Fe1—C5—C1	81.5 (2)	C9—Fe1—C10—C6	−118.5 (3)
C2—Fe1—C5—C1	37.61 (19)	C4—Fe1—C10—C6	167.43 (17)
C7—Fe1—C5—C1	−39.5 (6)	C18—C13—C14—F1	−179.7 (2)
C8—Fe1—C5—C1	171.1 (3)	C12—C13—C14—F1	1.4 (4)
C10—Fe1—C5—C1	−112.45 (19)	C18—C13—C14—C15	0.2 (4)
C6—Fe1—C5—C1	−71.4 (2)	C12—C13—C14—C15	−178.7 (3)
C9—Fe1—C5—C1	−154.93 (19)	F1—C14—C15—F2	−1.7 (4)
C4—Fe1—C5—C1	119.4 (3)	C13—C14—C15—F2	178.4 (2)
C3—Fe1—C6—C11	−68.3 (4)	F1—C14—C15—C16	179.7 (2)
C2—Fe1—C6—C11	−35.1 (3)	C13—C14—C15—C16	−0.2 (4)
C1—Fe1—C6—C11	7.5 (3)	F2—C15—C16—F3	3.0 (4)
C7—Fe1—C6—C11	−121.1 (3)	C14—C15—C16—F3	−178.4 (2)
C8—Fe1—C6—C11	−158.9 (3)	F2—C15—C16—C17	−178.2 (2)
C10—Fe1—C6—C11	120.0 (3)	C14—C15—C16—C17	0.4 (4)
C5—Fe1—C6—C11	47.6 (3)	F3—C16—C17—F4	−1.9 (4)
C9—Fe1—C6—C11	157.8 (3)	C15—C16—C17—F4	179.4 (3)
C4—Fe1—C6—C11	76.5 (5)	F3—C16—C17—C18	178.2 (2)
C3—Fe1—C6—C7	52.8 (3)	C15—C16—C17—C18	−0.6 (4)
C2—Fe1—C6—C7	86.0 (2)	F4—C17—C18—F5	1.2 (4)
C1—Fe1—C6—C7	128.66 (18)	C16—C17—C18—F5	−178.9 (2)
C8—Fe1—C6—C7	−37.81 (19)	F4—C17—C18—C13	−179.3 (2)
C10—Fe1—C6—C7	−118.9 (3)	C16—C17—C18—C13	0.6 (4)
C5—Fe1—C6—C7	168.71 (17)	C14—C13—C18—F5	179.1 (2)
C9—Fe1—C6—C7	−81.1 (2)	C12—C13—C18—F5	−2.0 (4)
C4—Fe1—C6—C7	−162.3 (4)	C14—C13—C18—C17	−0.4 (4)
C3—Fe1—C6—C10	171.8 (2)	C12—C13—C18—C17	178.5 (3)
C2—Fe1—C6—C10	−155.05 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10···F5^{i}	0.93	2.50	3.176 (3)	130

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+2.