

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

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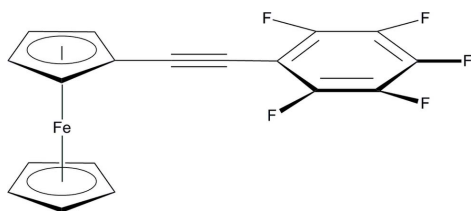
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Key indicators: single-crystal X-ray study; $T = 292$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.040; wR factor = 0.105; data-to-parameter ratio = 11.7.

The molecular structure of the title compound, $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{13}\text{H}_4\text{F}_5)]$, 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 $\text{C}-\text{H}\cdots\text{F}$ hydrogen bonds, $\text{C}-\text{F}\cdots\pi$ interactions between the pentafluorobenzene groups [$\text{F}\cdots$ centroid distances = 3.882 (2) and 3.884 (2) Å] and $\pi-\pi$ 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

$[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{13}\text{H}_4\text{F}_5)]$	$\gamma = 78.726$ (2) $^\circ$
$M_r = 376.10$	$V = 731.41$ (18) Å ³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 6.0767$ (9) Å	Mo $K\alpha$ radiation
$b = 10.7164$ (15) Å	$\mu = 1.08$ mm ⁻¹
$c = 12.6014$ (18) Å	$T = 292$ K
$\alpha = 65.725$ (2) $^\circ$	$0.30 \times 0.04 \times 0.02$ mm
$\beta = 89.364$ (3) $^\circ$	

Data collection

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

Refinement

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

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}10-\text{H}10\cdots\text{F}5^i$	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).

References

- Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Debroy, P. & Roy, S. (2007). *Coord. Chem. Rev.* **251**, 203–221.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Torres, J. C., Pilli, R. A., Vargas, M. D., Violante, F. A., Garden, S. J. & Pinto, A. C. (2002). *Tetrahedron*, **58**, 4487–4492.
- Valdebenito, C., Garland, M. T., Fuentealba, M. & Escobar, C. A. (2010). *Acta Cryst.* **E66**, m838.
- Zora, M., Açıkgöz, C., Tumay, T. A., Odabaşoğlu, M. & Büyükgüngör, O. (2006). *Acta Cryst.* **C62**, m327–m330.

supplementary materials

Acta Cryst. (2010). E66, m914 [doi:10.1107/S1600536810026772]

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

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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 \cdots F hydrogen bond between the ferrocenyl and pentafluorobenzene (Table 1), C—F \cdots π interactions between the pentafluorobenzene groups [F \cdots 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].

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(CH₃CO₂)₂ (40 mg, 0.2 mmol), Pd(PPh₃)₂Cl₂ (140 mg, 0.2 mmol) and ¹Pr₂NH (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 Na₂SO₄. 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.

Refinement

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

Figures

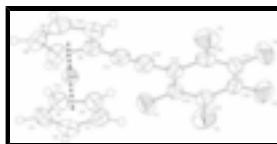


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

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

Crystal data

[Fe(C₅H₅)(C₁₃H₄F₅)]

Z = 2

supplementary materials

$M_r = 376.10$	$F(000) = 376$
Triclinic, $P\bar{1}$	$D_x = 1.708 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 6.0767 (9) \text{ \AA}$	Cell parameters from 1760 reflections
$b = 10.7164 (15) \text{ \AA}$	$\theta = 3.3\text{--}25.1^\circ$
$c = 12.6014 (18) \text{ \AA}$	$\mu = 1.08 \text{ mm}^{-1}$
$\alpha = 65.725 (2)^\circ$	$T = 292 \text{ K}$
$\beta = 89.364 (3)^\circ$	Plate, yellow
$\gamma = 78.726 (2)^\circ$	$0.30 \times 0.04 \times 0.02 \text{ mm}$
$V = 731.41 (18) \text{ \AA}^3$	

Data collection

Bruker SMART APEX CCD diffractometer	2169 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube graphite	$R_{\text{int}} = 0.021$
φ and ω scans	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 1.8^\circ$
4793 measured reflections	$h = -7 \rightarrow 7$
2533 independent reflections	$k = -12 \rightarrow 12$
	$l = -13 \rightarrow 14$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.105$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.0784P]$
2533 reflections	where $P = (F_o^2 + 2F_c^2)/3$
217 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.41 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.25 \text{ e \AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^2)

	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)

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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, °)

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)

supplementary materials

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)

supplementary materials

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 (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C10—H10 \cdots F5 ⁱ	0.93	2.50	3.176 (3)	130

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

Fig. 1

