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[6-(Hydroxymethyl)pyridin-2-yl]methyl ferrocene-1-carboxylate

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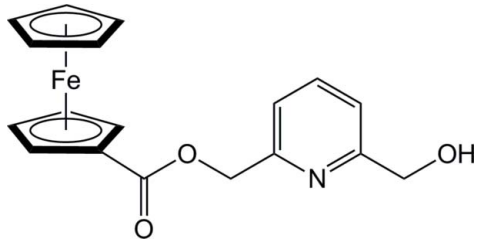
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.038; wR factor = 0.083; data-to-parameter ratio = 13.2.

The crystal structure of the title ferrocene derivative, $[Fe(C_5H_5)(C_{13}H_{12}NO_3)]$, shows strong intermolecular O—H···N hydrogen bonds between the alcohol function and the pyridine group of a neighbouring molecule, while the pyridine function forms another hydrogen bond with the alcohol function of another neighbouring molecule, resulting in the formation of chains along the *a*-axis direction.

Related literature

For analogous pyridinoferrocene derivatives and the synthesis of the title compound, see: Izumi *et al.* (1984, 1988). For a review on ferrocene derivatives as anticancer agents, see: Hillard & Jaouen (2011). For related structures, see: Auzias *et al.* (2008, 2009).



Experimental

Crystal data

$[Fe(C_5H_5)(C_{13}H_{12}NO_3)]$ M_r = 351.18
Tetragonal, $P4_12_12$
a = 7.5477 (3) Å
c = 53.351 (4) Å
V = 3039.3 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.01 mm^{-1}
T = 173 K
0.17 × 0.14 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
13026 measured reflections
2808 independent reflections
2092 reflections with $I > 2\sigma(I)$
R_{int} = 0.072

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.083
S = 0.86
2808 reflections
212 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}
Absolute structure: Flack (1983), 1024 Friedel pairs
Flack parameter: 0.02 (3)

Data collection: *SMART* (Bruker, 1999); cell refinement: *SMART* and *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FF2038).

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supporting information

Acta Cryst. (2011). E**67**, m1618 [doi:10.1107/S1600536811043972]

[6-(Hydroxymethyl)pyridin-2-yl]methyl ferrocene-1-carboxylate

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S1. Comment

Ferrocene derivatives are known to exert antiproliferative effects on cancers (Hillard & Jaouen, 2011) and, in this paper, the molecular structure of a ferrocene derivative, {6-(hydroxymethyl)pyridin-2-yl}methyl ferrocene-1-carboxylate, is presented. However, a biological evaluation was not possible due to the low water-solubility of the compound.

The title compound is obtained following a previsouly published procedure (Izumi *et al.*, 1984; Izumi *et al.*, 1988) using ferrocenoyl chloride and 2,6-pyridinedimethanol in the presence of triethylamine. After purification, the compound crystallizes in the tetragonal space group $P\,4_12_12$ with eight molecules per unit cell. These molecules are pilled along the *c* axis (*c* = 53.351 (4) Å). In the solid state, the ferrocene adopts an eclipsed conformation, and the pyridyl substituent is positionned perpendicular to the plane of the η^5-$C_5H_4COOCH_2$– moiety. Otherwise, the metrical parameters are normal and compare well to those of analogous functionalized-ferrocenyl molecules (Auzias *et al.*, 2008; Auzias *et al.*, 2009).

In the crystal packing, the pyridyl and the alcohol functions are involved in strong H-bonded interactions with two neighbouring symmetry-related molecules: The N—O separation being 2.827 (4) Å with the O—H···N angle being 159 (6)°.

S2. Experimental

Crystals suitable for X-ray diffraction analysis were obtained, after days, by slow diffusion of diethyl ether into a chloroform solution of the title complex.

S3. Refinement

All H atoms, except for OH, were included in calculated positions (C—H = 0.93 Å for C_{arom}, 0.97 Å for CH_2) and treated as riding atoms with the constraint $U_{iso}(H) = 1.2\,U_{eq}$(carrier) applied.

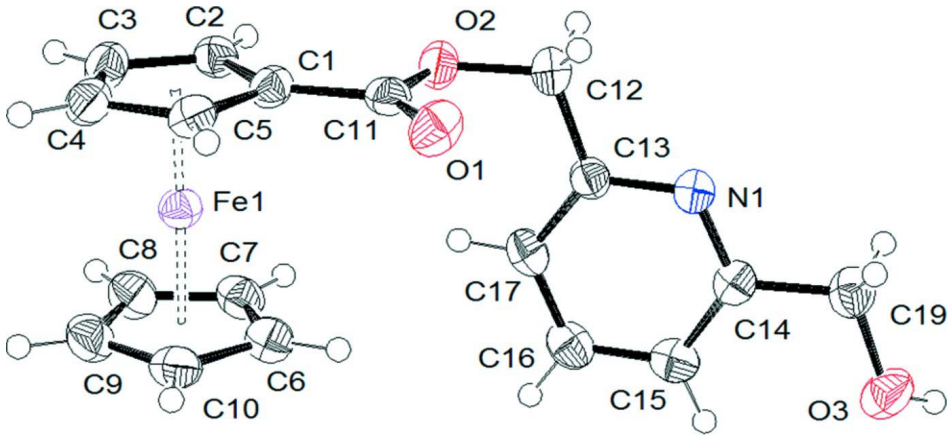

Figure 1

The molecular structure of {6-(hydroxymethyl)pyridin-2-yl}methyl ferrocene-1-carboxylate. Displacement ellipsoids are drawn at the 50% probability level.

[6-(Hydroxymethyl)pyridin-2-yl]methyl ferrocene-1-carboxylate

Crystal data

$[Fe(C_5H_5)(C_{13}H_{12}NO_3)]$
$M_r = 351.18$
Tetragonal, $P4_12_12$
Hall symbol: P 4abw 2nw
$a = 7.5477$ (3) Å
$c = 53.351$ (4) Å
$V = 3039.3$ (3) Å^3
$Z = 8$
$F(000) = 1456$
$D_x = 1.535$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9687 reflections
$\theta = 1.5$–$26.0°$
$\mu = 1.01$ mm^{-1}
$T = 173$ K
Block, orange
0.17 × 0.14 × 0.12 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω scans
13026 measured reflections
2808 independent reflections
2092 reflections with $I > 2\sigma(I)$
$R_{int} = 0.072$
$\theta_{max} = 25.6°$, $\theta_{min} = 1.5°$
$h = -9 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -64 \rightarrow 64$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.083$
$S = 0.86$
2808 reflections
212 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0458P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.57$ e Å^{-3}
Absolute structure: Flack (1983), 1024 Friedel pairs
Absolute structure parameter: 0.02 (3)

Special details

Experimental. A crystal was mounted at 173 K on a Bruker *SMART* CCD PLATFORM using Mo *Kα* graphite monochromated radiation. Image plate distance 70 mm, φ oscillation scans 0 - 200°, step $\Delta\varphi$ = 0.5°, 3 minutes per frame.

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.16190 (7)	0.78987 (6)	0.032064 (10)	0.03038 (14)
O2	−0.0794 (3)	0.8358 (3)	0.09355 (4)	0.0367 (6)
O1	−0.2404 (3)	0.9840 (3)	0.06481 (6)	0.0436 (7)
C11	−0.0980 (5)	0.9287 (5)	0.07208 (7)	0.0323 (8)
C7	0.1223 (5)	0.5232 (5)	0.03604 (7)	0.0393 (9)
H7	0.1192	0.4606	0.0510	0.047*
C1	0.0706 (5)	0.9566 (4)	0.05913 (7)	0.0307 (8)
C5	0.0887 (5)	1.0483 (5)	0.03606 (7)	0.0335 (8)
H5	−0.0017	1.1044	0.0273	0.040*
C9	0.2208 (5)	0.6541 (5)	−0.00017 (8)	0.0432 (10)
H9	0.2945	0.6926	−0.0130	0.052*
C4	0.2692 (5)	1.0391 (5)	0.02876 (8)	0.0375 (9)
H4	0.3180	1.0894	0.0144	0.045*
N1	−0.5056 (4)	0.6281 (4)	0.10764 (5)	0.0300 (7)
C13	−0.3422 (4)	0.6468 (4)	0.09774 (6)	0.0304 (8)
C14	−0.6050 (5)	0.4895 (5)	0.10050 (6)	0.0318 (9)
C17	−0.2723 (5)	0.5255 (5)	0.08130 (7)	0.0365 (9)
H17	−0.1574	0.5386	0.0753	0.044*
C10	0.0354 (5)	0.6827 (5)	0.00140 (7)	0.0400 (9)
H10	−0.0344	0.7431	−0.0101	0.048*
C2	0.2408 (5)	0.8887 (5)	0.06595 (7)	0.0318 (8)
H2	0.2673	0.8227	0.0802	0.038*
C16	−0.3757 (5)	0.3827 (5)	0.07373 (7)	0.0381 (10)
H16	−0.3321	0.3007	0.0623	0.046*
C15	−0.5450 (5)	0.3646 (5)	0.08355 (7)	0.0361 (9)
H15	−0.6167	0.2702	0.0788	0.043*
C3	0.3618 (5)	0.9408 (5)	0.04698 (8)	0.0379 (9)
H3	0.4821	0.9145	0.0466	0.046*
C8	0.2748 (6)	0.5564 (5)	0.02136 (8)	0.0426 (10)
H8	0.3897	0.5207	0.0251	0.051*
C19	−0.7864 (5)	0.4814 (5)	0.11208 (8)	0.0399 (10)
H19A	−0.7748	0.4622	0.1300	0.048*
H19B	−0.8458	0.5939	0.1096	0.048*

C6	−0.0237 (5)	0.6013 (5)	0.02401 (7)	0.0385 (9)
H6	−0.1398	0.6001	0.0298	0.046*
C12	−0.2403 (5)	0.8036 (5)	0.10734 (7)	0.0418 (9)
H12A	−0.3148	0.9081	0.1064	0.050*
H12B	−0.2110	0.7842	0.1248	0.050*
O3	−0.8909 (4)	0.3441 (4)	0.10162 (6)	0.0475 (7)
H3O	−0.935 (8)	0.248 (8)	0.1126 (13)	0.14 (3)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0306 (3)	0.0287 (3)	0.0318 (2)	0.0000 (2)	−0.0007 (2)	−0.0016 (2)
O2	0.0287 (13)	0.0459 (16)	0.0356 (14)	−0.0041 (12)	0.0036 (11)	0.0020 (13)
O1	0.0284 (16)	0.0444 (16)	0.0581 (18)	0.0058 (12)	−0.0066 (13)	0.0012 (14)
C11	0.033 (2)	0.029 (2)	0.035 (2)	−0.0008 (16)	−0.0008 (16)	−0.0083 (16)
C7	0.050 (3)	0.034 (2)	0.034 (2)	0.0004 (17)	0.0023 (18)	−0.0036 (17)
C1	0.025 (2)	0.031 (2)	0.036 (2)	−0.0003 (14)	−0.0020 (15)	−0.0020 (16)
C5	0.034 (2)	0.031 (2)	0.035 (2)	−0.0041 (15)	−0.0046 (16)	0.0000 (16)
C9	0.051 (3)	0.038 (2)	0.040 (2)	−0.001 (2)	0.0090 (18)	−0.0070 (19)
C4	0.035 (2)	0.038 (2)	0.039 (2)	−0.0072 (16)	−0.0006 (17)	0.0016 (17)
N1	0.0288 (17)	0.0290 (18)	0.0323 (16)	0.0008 (13)	0.0012 (13)	0.0023 (13)
C13	0.0292 (19)	0.0329 (19)	0.0293 (17)	0.0014 (17)	0.0016 (14)	−0.0011 (14)
C14	0.032 (2)	0.031 (2)	0.033 (2)	−0.0004 (15)	−0.0016 (15)	0.0056 (16)
C17	0.036 (2)	0.039 (2)	0.034 (2)	0.0064 (17)	0.0060 (17)	−0.0020 (17)
C10	0.046 (3)	0.040 (2)	0.034 (2)	−0.0031 (18)	−0.0052 (17)	−0.0045 (19)
C2	0.032 (2)	0.035 (2)	0.0285 (18)	−0.0001 (15)	−0.0023 (15)	−0.0006 (15)
C16	0.047 (3)	0.030 (2)	0.038 (2)	0.0062 (17)	0.0044 (18)	0.0002 (16)
C15	0.047 (2)	0.028 (2)	0.033 (2)	−0.0003 (18)	−0.0017 (17)	0.0027 (16)
C3	0.028 (2)	0.041 (2)	0.045 (2)	−0.0030 (18)	0.0017 (17)	−0.0012 (17)
C8	0.044 (2)	0.042 (2)	0.041 (2)	0.0041 (19)	0.0026 (19)	−0.0038 (18)
C19	0.042 (2)	0.036 (2)	0.042 (2)	−0.0028 (18)	0.0048 (19)	0.0052 (17)
C6	0.041 (2)	0.037 (2)	0.037 (2)	0.0010 (17)	−0.0001 (18)	−0.0021 (17)
C12	0.036 (2)	0.051 (3)	0.039 (2)	−0.0074 (17)	0.0099 (16)	−0.0056 (19)
O3	0.0446 (17)	0.0500 (18)	0.0478 (17)	−0.0159 (14)	−0.0041 (13)	0.0078 (15)

Geometric parameters (Å, º)

Fe1—C1	2.035 (3)	C4—H4	0.9300
Fe1—C5	2.038 (4)	N1—C14	1.342 (4)
Fe1—C8	2.039 (4)	N1—C13	1.349 (4)
Fe1—C6	2.042 (4)	C13—C17	1.373 (5)
Fe1—C2	2.045 (3)	C13—C12	1.502 (5)
Fe1—C7	2.046 (4)	C14—C15	1.382 (5)
Fe1—C9	2.051 (4)	C14—C19	1.504 (5)
Fe1—C3	2.051 (4)	C17—C16	1.390 (5)
Fe1—C4	2.056 (3)	C17—H17	0.9300
Fe1—C10	2.060 (4)	C10—C6	1.425 (5)
O2—C11	1.350 (4)	C10—H10	0.9300

O2—C12	1.440 (4)	C2—C3	1.419 (5)
O1—C11	1.217 (4)	C2—H2	0.9300
C11—C1	1.464 (5)	C16—C15	1.388 (5)
C7—C6	1.404 (5)	C16—H16	0.9300
C7—C8	1.414 (5)	C15—H15	0.9300
C7—H7	0.9300	C3—H3	0.9300
C1—C5	1.419 (5)	C8—H8	0.9300
C1—C2	1.430 (5)	C19—O3	1.416 (4)
C5—C4	1.418 (5)	C19—H19A	0.9700
C5—H5	0.9300	C19—H19B	0.9700
C9—C10	1.418 (5)	C6—H6	0.9300
C9—C8	1.425 (6)	C12—H12A	0.9700
C9—H9	0.9300	C12—H12B	0.9700
C4—C3	1.408 (5)	O3—H3O	0.99 (6)

C1—Fe1—C5	40.77 (13)	C8—C9—Fe1	69.2 (2)
C1—Fe1—C8	150.96 (15)	C10—C9—H9	125.9
C5—Fe1—C8	165.83 (15)	C8—C9—H9	125.9
C1—Fe1—C6	110.37 (15)	Fe1—C9—H9	126.3
C5—Fe1—C6	120.19 (15)	C3—C4—C5	108.2 (4)
C8—Fe1—C6	67.99 (16)	C3—C4—Fe1	69.8 (2)
C1—Fe1—C2	41.02 (13)	C5—C4—Fe1	69.07 (19)
C5—Fe1—C2	68.73 (14)	C3—C4—H4	125.9
C8—Fe1—C2	116.19 (16)	C5—C4—H4	125.9
C6—Fe1—C2	129.80 (14)	Fe1—C4—H4	126.9
C1—Fe1—C7	119.02 (14)	C14—N1—C13	118.7 (3)
C5—Fe1—C7	152.99 (14)	N1—C13—C17	122.1 (3)
C8—Fe1—C7	40.51 (14)	N1—C13—C12	114.6 (3)
C6—Fe1—C7	40.19 (15)	C17—C13—C12	123.1 (3)
C2—Fe1—C7	108.06 (15)	N1—C14—C15	122.3 (3)
C1—Fe1—C9	167.76 (15)	N1—C14—C19	115.1 (3)
C5—Fe1—C9	128.65 (16)	C15—C14—C19	122.6 (3)
C8—Fe1—C9	40.78 (15)	C13—C17—C16	119.1 (4)
C6—Fe1—C9	67.92 (15)	C13—C17—H17	120.4
C2—Fe1—C9	149.40 (15)	C16—C17—H17	120.4
C7—Fe1—C9	68.11 (15)	C9—C10—C6	107.1 (4)
C1—Fe1—C3	68.30 (15)	C9—C10—Fe1	69.5 (2)
C5—Fe1—C3	68.11 (14)	C6—C10—Fe1	69.0 (2)
C8—Fe1—C3	106.35 (16)	C9—C10—H10	126.5
C6—Fe1—C3	166.67 (15)	C6—C10—H10	126.5
C2—Fe1—C3	40.54 (14)	Fe1—C10—H10	126.6
C7—Fe1—C3	127.87 (15)	C3—C2—C1	107.3 (3)
C9—Fe1—C3	116.32 (15)	C3—C2—Fe1	70.0 (2)
C1—Fe1—C4	68.18 (15)	C1—C2—Fe1	69.1 (2)
C5—Fe1—C4	40.54 (14)	C3—C2—H2	126.4
C8—Fe1—C4	127.05 (15)	C1—C2—H2	126.4
C6—Fe1—C4	152.84 (16)	Fe1—C2—H2	126.1
C2—Fe1—C4	68.10 (15)	C15—C16—C17	118.9 (4)

C7—Fe1—C4	165.19 (15)	C15—C16—H16	120.5
C9—Fe1—C4	107.45 (16)	C17—C16—H16	120.5
C3—Fe1—C4	40.10 (15)	C14—C15—C16	118.8 (3)
C1—Fe1—C10	130.51 (16)	C14—C15—H15	120.6
C5—Fe1—C10	109.47 (16)	C16—C15—H15	120.6
C8—Fe1—C10	68.39 (17)	C4—C3—C2	108.6 (3)
C6—Fe1—C10	40.65 (14)	C4—C3—Fe1	70.1 (2)
C2—Fe1—C10	168.74 (14)	C2—C3—Fe1	69.5 (2)
C7—Fe1—C10	68.17 (16)	C4—C3—H3	125.7
C9—Fe1—C10	40.37 (15)	C2—C3—H3	125.7
C3—Fe1—C10	150.13 (16)	Fe1—C3—H3	126.3
C4—Fe1—C10	118.30 (16)	C7—C8—C9	107.8 (4)
C11—O2—C12	115.7 (3)	C7—C8—Fe1	70.0 (2)
O1—C11—O2	122.7 (3)	C9—C8—Fe1	70.0 (2)
O1—C11—C1	124.6 (4)	C7—C8—H8	126.1
O2—C11—C1	112.6 (3)	C9—C8—H8	126.1
C6—C7—C8	108.1 (3)	Fe1—C8—H8	125.4
C6—C7—Fe1	69.8 (2)	O3—C19—C14	112.0 (3)
C8—C7—Fe1	69.5 (2)	O3—C19—H19A	109.2
C6—C7—H7	125.9	C14—C19—H19A	109.2
C8—C7—H7	125.9	O3—C19—H19B	109.2
Fe1—C7—H7	126.4	C14—C19—H19B	109.2
C5—C1—C2	108.0 (3)	H19A—C19—H19B	107.9
C5—C1—C11	124.3 (3)	C7—C6—C10	108.8 (4)
C2—C1—C11	127.6 (3)	C7—C6—Fe1	70.0 (2)
C5—C1—Fe1	69.7 (2)	C10—C6—Fe1	70.3 (2)
C2—C1—Fe1	69.8 (2)	C7—C6—H6	125.6
C11—C1—Fe1	122.7 (2)	C10—C6—H6	125.6
C4—C5—C1	107.9 (3)	Fe1—C6—H6	125.6
C4—C5—Fe1	70.4 (2)	O2—C12—C13	113.0 (3)
C1—C5—Fe1	69.5 (2)	O2—C12—H12A	109.0
C4—C5—H5	126.1	C13—C12—H12A	109.0
C1—C5—H5	126.1	O2—C12—H12B	109.0
Fe1—C5—H5	125.6	C13—C12—H12B	109.0
C10—C9—C8	108.2 (4)	H12A—C12—H12B	107.8
C10—C9—Fe1	70.2 (2)	C19—O3—H3O	119 (4)

C12—O2—C11—O1	0.8 (5)	C8—C9—C10—Fe1	58.9 (3)
C12—O2—C11—C1	179.9 (3)	C1—Fe1—C10—C9	168.4 (2)
C1—Fe1—C7—C6	87.7 (2)	C5—Fe1—C10—C9	127.4 (2)
C5—Fe1—C7—C6	52.7 (4)	C8—Fe1—C10—C9	−37.7 (2)
C8—Fe1—C7—C6	−119.4 (3)	C6—Fe1—C10—C9	−118.6 (4)
C2—Fe1—C7—C6	131.1 (2)	C2—Fe1—C10—C9	−153.9 (7)
C9—Fe1—C7—C6	−81.3 (2)	C7—Fe1—C10—C9	−81.4 (3)
C3—Fe1—C7—C6	171.7 (2)	C3—Fe1—C10—C9	47.6 (4)
C4—Fe1—C7—C6	−156.5 (6)	C4—Fe1—C10—C9	83.8 (3)
C10—Fe1—C7—C6	−37.6 (2)	C1—Fe1—C10—C6	−73.0 (3)
C1—Fe1—C7—C8	−152.9 (2)	C5—Fe1—C10—C6	−114.0 (2)

C5—Fe1—C7—C8	172.1 (3)	C8—Fe1—C10—C6	80.9 (3)
C6—Fe1—C7—C8	119.4 (3)	C2—Fe1—C10—C6	−35.2 (9)
C2—Fe1—C7—C8	−109.5 (2)	C7—Fe1—C10—C6	37.2 (2)
C9—Fe1—C7—C8	38.2 (2)	C9—Fe1—C10—C6	118.6 (4)
C3—Fe1—C7—C8	−68.8 (3)	C3—Fe1—C10—C6	166.3 (3)
C4—Fe1—C7—C8	−37.0 (7)	C4—Fe1—C10—C6	−157.5 (2)
C10—Fe1—C7—C8	81.8 (3)	C5—C1—C2—C3	0.3 (4)
O1—C11—C1—C5	−1.6 (6)	C11—C1—C2—C3	176.2 (3)
O2—C11—C1—C5	179.3 (3)	Fe1—C1—C2—C3	59.8 (2)
O1—C11—C1—C2	−176.8 (4)	C5—C1—C2—Fe1	−59.5 (2)
O2—C11—C1—C2	4.1 (5)	C11—C1—C2—Fe1	116.3 (3)
O1—C11—C1—Fe1	−88.2 (4)	C1—Fe1—C2—C3	−118.5 (3)
O2—C11—C1—Fe1	92.8 (3)	C5—Fe1—C2—C3	−80.8 (2)
C8—Fe1—C1—C5	165.9 (3)	C8—Fe1—C2—C3	84.7 (3)
C6—Fe1—C1—C5	−113.0 (2)	C6—Fe1—C2—C3	167.0 (2)
C2—Fe1—C1—C5	119.1 (3)	C7—Fe1—C2—C3	127.7 (2)
C7—Fe1—C1—C5	−156.5 (2)	C9—Fe1—C2—C3	50.4 (4)
C9—Fe1—C1—C5	−33.4 (8)	C4—Fe1—C2—C3	−37.0 (2)
C3—Fe1—C1—C5	81.2 (2)	C10—Fe1—C2—C3	−163.7 (7)
C4—Fe1—C1—C5	37.9 (2)	C5—Fe1—C2—C1	37.74 (19)
C10—Fe1—C1—C5	−71.4 (3)	C8—Fe1—C2—C1	−156.8 (2)
C5—Fe1—C1—C2	−119.1 (3)	C6—Fe1—C2—C1	−74.5 (3)
C8—Fe1—C1—C2	46.8 (4)	C7—Fe1—C2—C1	−113.7 (2)
C6—Fe1—C1—C2	127.9 (2)	C9—Fe1—C2—C1	168.9 (3)
C7—Fe1—C1—C2	84.4 (2)	C3—Fe1—C2—C1	118.5 (3)
C9—Fe1—C1—C2	−152.5 (7)	C4—Fe1—C2—C1	81.5 (2)
C3—Fe1—C1—C2	−37.9 (2)	C10—Fe1—C2—C1	−45.2 (9)
C4—Fe1—C1—C2	−81.3 (2)	C13—C17—C16—C15	−1.7 (6)
C10—Fe1—C1—C2	169.5 (2)	N1—C14—C15—C16	0.4 (5)
C5—Fe1—C1—C11	118.5 (4)	C19—C14—C15—C16	179.8 (3)
C8—Fe1—C1—C11	−75.6 (4)	C17—C16—C15—C14	0.1 (6)
C6—Fe1—C1—C11	5.5 (3)	C5—C4—C3—C2	−0.5 (4)
C2—Fe1—C1—C11	−122.4 (4)	Fe1—C4—C3—C2	−59.0 (3)
C7—Fe1—C1—C11	−38.0 (4)	C5—C4—C3—Fe1	58.5 (2)
C9—Fe1—C1—C11	85.1 (8)	C1—C2—C3—C4	0.1 (4)
C3—Fe1—C1—C11	−160.3 (3)	Fe1—C2—C3—C4	59.4 (3)
C4—Fe1—C1—C11	156.3 (3)	C1—C2—C3—Fe1	−59.3 (2)
C10—Fe1—C1—C11	47.1 (4)	C1—Fe1—C3—C4	−81.5 (2)
C2—C1—C5—C4	−0.6 (4)	C5—Fe1—C3—C4	−37.4 (2)
C11—C1—C5—C4	−176.7 (3)	C8—Fe1—C3—C4	128.8 (2)
Fe1—C1—C5—C4	−60.2 (3)	C6—Fe1—C3—C4	−168.3 (6)
C2—C1—C5—Fe1	59.6 (2)	C2—Fe1—C3—C4	−119.8 (3)
C11—C1—C5—Fe1	−116.4 (3)	C7—Fe1—C3—C4	167.9 (2)
C1—Fe1—C5—C4	118.7 (3)	C9—Fe1—C3—C4	86.1 (3)
C8—Fe1—C5—C4	−32.4 (7)	C10—Fe1—C3—C4	53.8 (4)
C6—Fe1—C5—C4	−154.6 (2)	C1—Fe1—C3—C2	38.4 (2)
C2—Fe1—C5—C4	80.8 (2)	C5—Fe1—C3—C2	82.4 (2)
C7—Fe1—C5—C4	169.0 (3)	C8—Fe1—C3—C2	−111.4 (2)

C9—Fe1—C5—C4	−69.9 (3)	C6—Fe1—C3—C2	−48.5 (7)
C3—Fe1—C5—C4	37.0 (2)	C7—Fe1—C3—C2	−72.2 (3)
C10—Fe1—C5—C4	−111.1 (2)	C9—Fe1—C3—C2	−154.1 (2)
C8—Fe1—C5—C1	−151.1 (6)	C4—Fe1—C3—C2	119.8 (3)
C6—Fe1—C5—C1	86.7 (2)	C10—Fe1—C3—C2	173.7 (3)
C2—Fe1—C5—C1	−38.0 (2)	C6—C7—C8—C9	−0.8 (4)
C7—Fe1—C5—C1	50.2 (4)	Fe1—C7—C8—C9	−60.1 (3)
C9—Fe1—C5—C1	171.4 (2)	C6—C7—C8—Fe1	59.3 (3)
C3—Fe1—C5—C1	−81.7 (2)	C10—C9—C8—C7	0.6 (4)
C4—Fe1—C5—C1	−118.7 (3)	Fe1—C9—C8—C7	60.1 (3)
C10—Fe1—C5—C1	130.2 (2)	C10—C9—C8—Fe1	−59.5 (3)
C1—Fe1—C9—C10	−46.3 (8)	C1—Fe1—C8—C7	55.3 (4)
C5—Fe1—C9—C10	−73.6 (3)	C5—Fe1—C8—C7	−165.3 (6)
C8—Fe1—C9—C10	119.5 (3)	C6—Fe1—C8—C7	−37.3 (2)
C6—Fe1—C9—C10	38.1 (2)	C2—Fe1—C8—C7	87.5 (2)
C2—Fe1—C9—C10	170.3 (3)	C9—Fe1—C8—C7	−118.6 (3)
C7—Fe1—C9—C10	81.6 (2)	C3—Fe1—C8—C7	129.9 (2)
C3—Fe1—C9—C10	−155.8 (2)	C4—Fe1—C8—C7	168.9 (2)
C4—Fe1—C9—C10	−113.4 (2)	C10—Fe1—C8—C7	−81.3 (2)
C1—Fe1—C9—C8	−165.8 (6)	C1—Fe1—C8—C9	173.8 (3)
C5—Fe1—C9—C8	166.8 (2)	C5—Fe1—C8—C9	−46.7 (7)
C6—Fe1—C9—C8	−81.4 (2)	C6—Fe1—C8—C9	81.3 (2)
C2—Fe1—C9—C8	50.7 (4)	C2—Fe1—C8—C9	−154.0 (2)
C7—Fe1—C9—C8	−37.9 (2)	C7—Fe1—C8—C9	118.6 (3)
C3—Fe1—C9—C8	84.7 (3)	C3—Fe1—C8—C9	−111.5 (2)
C4—Fe1—C9—C8	127.0 (2)	C4—Fe1—C8—C9	−72.6 (3)
C10—Fe1—C9—C8	−119.5 (3)	C10—Fe1—C8—C9	37.3 (2)
C1—C5—C4—C3	0.7 (4)	N1—C14—C19—O3	173.3 (3)
Fe1—C5—C4—C3	−58.9 (3)	C15—C14—C19—O3	−6.2 (5)
C1—C5—C4—Fe1	59.7 (2)	C8—C7—C6—C10	0.7 (4)
C1—Fe1—C4—C3	81.8 (3)	Fe1—C7—C6—C10	59.9 (3)
C5—Fe1—C4—C3	119.9 (3)	C8—C7—C6—Fe1	−59.1 (3)
C8—Fe1—C4—C3	−69.6 (3)	C9—C10—C6—C7	−0.4 (4)
C6—Fe1—C4—C3	174.1 (3)	Fe1—C10—C6—C7	−59.7 (3)
C2—Fe1—C4—C3	37.4 (2)	C9—C10—C6—Fe1	59.3 (3)
C7—Fe1—C4—C3	−40.3 (7)	C1—Fe1—C6—C7	−111.3 (2)
C9—Fe1—C4—C3	−110.4 (2)	C5—Fe1—C6—C7	−155.3 (2)
C10—Fe1—C4—C3	−152.8 (2)	C8—Fe1—C6—C7	37.6 (2)
C1—Fe1—C4—C5	−38.1 (2)	C2—Fe1—C6—C7	−68.8 (3)
C8—Fe1—C4—C5	170.5 (2)	C9—Fe1—C6—C7	81.8 (2)
C6—Fe1—C4—C5	54.3 (5)	C3—Fe1—C6—C7	−29.5 (8)
C2—Fe1—C4—C5	−82.4 (2)	C4—Fe1—C6—C7	167.1 (3)
C7—Fe1—C4—C5	−160.1 (5)	C10—Fe1—C6—C7	119.6 (3)
C9—Fe1—C4—C5	129.8 (2)	C1—Fe1—C6—C10	129.1 (2)
C3—Fe1—C4—C5	−119.9 (3)	C5—Fe1—C6—C10	85.1 (3)
C10—Fe1—C4—C5	87.3 (3)	C8—Fe1—C6—C10	−82.0 (3)
C14—N1—C13—C17	−2.3 (5)	C2—Fe1—C6—C10	171.6 (2)
C14—N1—C13—C12	−178.8 (3)	C7—Fe1—C6—C10	−119.6 (3)

C13—N1—C14—C15	0.6 (5)	C9—Fe1—C6—C10	−37.8 (2)
C13—N1—C14—C19	−178.8 (3)	C3—Fe1—C6—C10	−149.1 (6)
N1—C13—C17—C16	2.8 (5)	C4—Fe1—C6—C10	47.5 (5)
C12—C13—C17—C16	179.0 (4)	C11—O2—C12—C13	82.9 (4)
C8—C9—C10—C6	−0.1 (4)	N1—C13—C12—O2	−170.6 (3)
Fe1—C9—C10—C6	−59.0 (3)	C17—C13—C12—O2	13.0 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3o···N1^{i}	0.99 (6)	1.88 (7)	2.827 (4)	159 (6)

Symmetry code: (i) −*x*−3/2, *y*−1/2, −*z*+1/4.