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Key indicators

Single-crystal X-ray study
 T = 160 K
 Mean $\sigma(\text{C}-\text{C}) = 0.011 \text{ \AA}$
 R factor = 0.035
 wR factor = 0.079
 Data-to-parameter ratio = 6.8

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

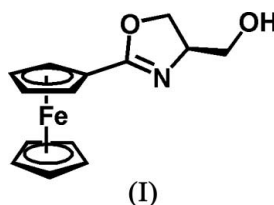
(R)-2-Ferrocenyl-4-hydroxymethyl-4,5-dihydro-1,3-oxazole

The title compound, $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_9\text{H}_{10}\text{NO}_2)]$, was prepared from ferrocenecarboxylic acid and serine. In the crystal structure, molecules are arranged in chains with an intermolecular hydrogen bond between hydroxy groups and N atoms.

Received 3 February 2006
 Accepted 27 February 2006

Comment

A series of serine-derived oxazoles has been shown to be effective in asymmetric alkylation reactions, and hence their crystal structures are of interest (Jones & Richards, 2004). As representatives of the general amino alcohol class of ligands for these reactions, we have an interest in understanding their non-linear catalytic characteristics. A single-crystal X-ray structure has been reported for a related compound, *viz.* (4*S*)-4-(1-hydroxy-1-methylethyl)-2-ferrocenyl-4,5-dihydro-1,3-oxazole monohydrate (Chesney *et al.*, 1998).



The structure of the title compound, (I) (Fig. 1), reveals that the two cyclopentadienyl rings of ferrocene deviate by only four degrees from a fully eclipsed conformation. The torsion angle $\text{C}1-\text{C}1c-\text{C}2c-\text{C}11$ (where $\text{C}1c$ and $\text{C}2c$ are the cyclopentadiene ring centroids) is $-3.5 (6)^\circ$. The oxazoline ring is almost coplanar with the cyclopentadienyl ring to which it is attached [interplanar angle = $9.2 (5)^\circ$ and $\text{C}2-\text{C}1-\text{C}6-\text{O}1 = -6.3 (10)^\circ$], the O rather than the N atom being slightly closer to iron. The oxazoline hydroxymethyl substituent is oriented away from the iron-cyclopentadienyl group of ferrocene. Significantly, the opposite rotamer, with respect to rotation about the ferrocene-oxazoline $\text{C}-\text{C}$ σ -bond, was observed in the structure reported by Chesney *et al.* (1998). This contains a larger 1-hydroxy-1-methylethoxyoxazoline substituent, and in both cases the hydroxy group is oriented over the oxazoline ring; in the present structure, $\text{N}1-\text{C}8-\text{C}9-\text{O}2 = -73.7 (7)^\circ$.

Experimental

LiAlH_4 (68 mg, 1.797 mmol, 1.1 equivalent) was added to a solution of (S)-4-carbomethoxy-2-ferrocenyl-1,3-oxazoline (513 mg, 1.634 mmol) in diethyl ether (15 ml) cooled to 273 K. After stirring for 15 min, ethyl acetate (25 ml) was added followed by water (38 ml), and the organic layer was then separated, dried (MgSO_4),

filtered and concentrated *in vacuo* to give the crude alcohol as an orange solid. The crude solid was recrystallized from dichloromethane and hexane (*ca* 1:1) to give the pure oxazoline [434 mg, 93%; m.p. 390–392 K (literature 390–392 K)]. ¹H NMR (CDCl₃): δ 3.59 (1H, *dd*, *J* = 11.4, 3.7 Hz, OCHH) and 3.86 (1H, *dd*, *J* = 11.4, 3.2 Hz OCHH), 4.16 (5H, *s*, Cp), 4.18–4.40 (5H, *m*, OCH₂ + CHN + Cp × 2), 4.72 (2H, *m*, Cp).

Crystal data

[Fe(C₅H₅)(C₉H₁₀NO₂)]
M_r = 285.12
 Monoclinic, *P*₂₁
a = 5.808 (4) Å
b = 7.557 (3) Å
c = 13.716 (8) Å
 β = 92.39 (6)°
V = 601.5 (6) Å³
Z = 2
D_x = 1.574 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 25 reflections
 θ = 9.9–13.2°
 μ = 1.25 mm⁻¹
T = 160 (2) K
 Prism, orange
 0.30 × 0.13 × 0.08 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 ω/2θ scans
 Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.706, *T_{max}* = 0.912
 1305 measured reflections
 1137 independent reflections
 877 reflections with *I* > 2σ(*I*)
R_{int} = 0.033
 θ_{max} = 25.0°
h = -1 → 6
k = 0 → 8
l = -16 → 16
 2 standard reflections every 100 reflections
 intensity decay: 5%

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.035
wR(*F*²) = 0.079
S = 1.03
 1137 reflections
 168 parameters
 H atoms treated by a mixture of independent and constrained refinement
w = 1/[σ²(*F_o*²) + (0.0336*P*)²]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.54 e Å⁻³
 Δρ_{min} = -0.37 e Å⁻³
 Absolute structure: Flack (1983), 171 Friedel Pairs
 Flack parameter: 0.01 (4)

Table 1

Selected torsion angles (°).

C2–C1–C6–O1	-6.3 (10)	N1–C8–C9–O2	-73.7 (7)
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Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
O2–H20...N1 ⁱ	0.87 (7)	2.02 (8)	2.877 (7)	165 (7)

Symmetry code: (i) -*x* + 1, *y* - ½, -*z* + 1.

H atoms were treated as riding atoms [C–H = 0.95 and 0.99 Å; *U_{iso}*(H) = 1.2*U_{eq}*(C)], except for H20, which was refined freely with an isotropic displacement parameter.

Data collection: *CAD-4/PC* (Enraf–Nonius, 1994); cell refinement: *CAD-4/PC*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

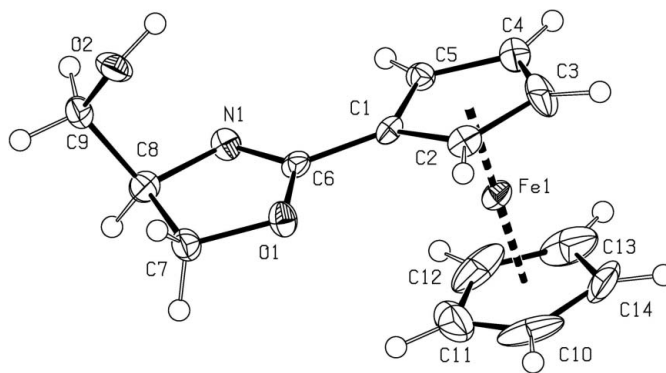


Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

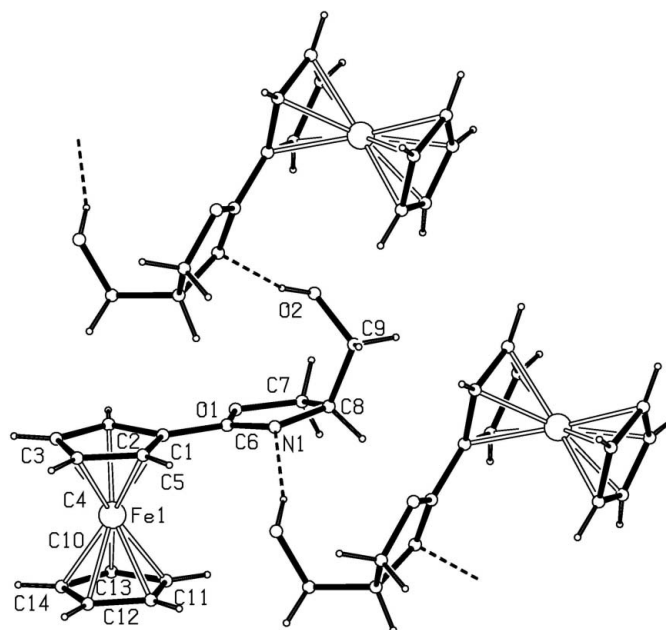


Figure 2

The polymeric assembly of (I), involving hydrogen-bonded (dashed lines) oxazole groups.

The authors thank Queen Mary University of London for financial support.

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supporting information

Acta Cryst. (2006). E62, m719–m720 [https://doi.org/10.1107/S1600536806006982]

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[Fe(C₅H₅)(C₉H₁₀NO₂)]

$M_r = 285.12$

Monoclinic, $P2_1$

Hall symbol: P 2y b

$a = 5.808$ (4) Å

$b = 7.557$ (3) Å

$c = 13.716$ (8) Å

$\beta = 92.39$ (6)°

$V = 601.5$ (6) Å³

$Z = 2$

$F(000) = 296$

$D_x = 1.574$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 9.9$ – 13.2 °

$\mu = 1.25$ mm⁻¹

$T = 160$ K

Prism, orange

$0.30 \times 0.13 \times 0.08$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

non-profiled $\omega/2\theta$ scans

Absorption correction: ψ scan

(North *et al.*, 1968)

$T_{\min} = 0.706$, $T_{\max} = 0.912$

1305 measured reflections

1137 independent reflections

877 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 3.1$ °

$h = -1 \rightarrow 6$

$k = 0 \rightarrow 8$

$l = -16 \rightarrow 16$

2 standard reflections every 100 reflections

intensity decay: 5%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.079$

$S = 1.03$

1137 reflections

168 parameters

1 restraint

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

$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.54$ e Å⁻³

$\Delta\rho_{\min} = -0.37$ e Å⁻³

Absolute structure: Flack (1983), 171 Friedel
Pairs

Absolute structure parameter: 0.01 (4)

Special details

Experimental. Number of psi-scan sets used was 3 Theta correction was applied. Averaged transmission function was used. No Fourier smoothing was applied.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6839 (10)	0.0630 (10)	0.6919 (4)	0.0169 (15)
C2	0.8278 (11)	-0.0481 (10)	0.7527 (5)	0.0192 (15)
H2	0.9815	-0.0823	0.7409	0.023*
C3	0.7001 (17)	-0.0974 (13)	0.8332 (7)	0.031 (3)
H3	0.7536	-0.1708	0.8857	0.037*
C4	0.4774 (12)	-0.0190 (11)	0.8232 (5)	0.0254 (16)
H4	0.3566	-0.0303	0.8674	0.030*
C5	0.4693 (10)	0.0788 (9)	0.7353 (4)	0.0177 (15)
H5	0.3407	0.1441	0.7097	0.021*
C6	0.7433 (9)	0.1413 (10)	0.5996 (4)	0.0171 (18)
C7	0.9844 (10)	0.2045 (11)	0.4816 (4)	0.0221 (18)
H7A	1.0478	0.1224	0.4333	0.026*
H7B	1.0858	0.3095	0.4879	0.026*
C8	0.7372 (10)	0.2586 (10)	0.4514 (4)	0.0208 (15)
H8	0.7314	0.3880	0.4362	0.025*
C9	0.6402 (11)	0.1529 (12)	0.3645 (4)	0.0231 (16)
H9A	0.4704	0.1659	0.3605	0.028*
H9B	0.7012	0.2020	0.3039	0.028*
C10	1.0133 (12)	0.3030 (13)	0.8785 (7)	0.047 (3)
H10	1.1679	0.2662	0.8708	0.056*
C11	0.8812 (19)	0.4114 (13)	0.8152 (6)	0.052 (3)
H11	0.9322	0.4623	0.7566	0.063*
C12	0.664 (2)	0.4326 (15)	0.8517 (9)	0.052 (3)
H12	0.5396	0.4982	0.8227	0.063*
C13	0.6638 (14)	0.3415 (15)	0.9372 (7)	0.053 (3)
H13	0.5367	0.3357	0.9785	0.064*
C14	0.8715 (16)	0.2591 (12)	0.9560 (6)	0.043 (2)
H14	0.9120	0.1866	1.0106	0.052*
Fe1	0.72777 (14)	0.1715 (2)	0.82749 (6)	0.0192 (2)
N1	0.6050 (8)	0.2214 (7)	0.5395 (3)	0.0196 (14)
O1	0.9634 (7)	0.1180 (6)	0.5750 (3)	0.0209 (11)
O2	0.6970 (8)	-0.0304 (7)	0.3711 (4)	0.0269 (11)
H20	0.610 (11)	-0.094 (11)	0.408 (5)	0.04 (2)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.016 (3)	0.019 (4)	0.015 (3)	0.001 (3)	-0.004 (3)	-0.002 (3)
C2	0.018 (3)	0.017 (4)	0.023 (4)	0.005 (3)	0.001 (3)	-0.006 (3)
C3	0.049 (7)	0.015 (5)	0.029 (5)	0.003 (4)	0.005 (5)	0.011 (4)
C4	0.026 (4)	0.028 (4)	0.022 (4)	-0.001 (3)	0.000 (3)	0.003 (3)
C5	0.018 (3)	0.018 (4)	0.017 (3)	-0.001 (3)	0.002 (3)	-0.002 (3)
C6	0.016 (3)	0.021 (5)	0.014 (3)	-0.002 (3)	0.001 (2)	-0.005 (3)
C7	0.021 (3)	0.024 (5)	0.022 (3)	0.000 (3)	0.001 (3)	0.005 (3)
C8	0.023 (4)	0.017 (3)	0.022 (4)	0.002 (3)	-0.002 (3)	0.000 (3)
C9	0.031 (3)	0.020 (4)	0.018 (3)	-0.004 (4)	0.000 (2)	0.004 (4)
C10	0.013 (4)	0.053 (6)	0.075 (7)	-0.003 (4)	0.003 (4)	-0.046 (5)
C11	0.086 (8)	0.044 (6)	0.028 (5)	-0.032 (6)	0.015 (6)	-0.006 (4)
C12	0.060 (7)	0.043 (7)	0.051 (7)	0.011 (6)	-0.027 (6)	-0.029 (6)
C13	0.034 (5)	0.079 (8)	0.047 (6)	-0.016 (5)	0.014 (4)	-0.040 (6)
C14	0.069 (6)	0.036 (5)	0.024 (4)	-0.010 (5)	-0.025 (4)	-0.002 (4)
Fe1	0.0192 (4)	0.0216 (4)	0.0165 (4)	0.0002 (7)	-0.0009 (3)	-0.0051 (7)
N1	0.021 (3)	0.019 (4)	0.019 (3)	0.002 (2)	0.004 (2)	0.000 (2)
O1	0.020 (2)	0.025 (3)	0.019 (2)	0.0050 (18)	0.0040 (19)	0.0033 (18)
O2	0.030 (3)	0.020 (3)	0.031 (3)	-0.009 (2)	0.006 (2)	0.002 (2)

Geometric parameters (\AA , $^\circ$)

C1—C5	1.408 (8)	C8—C9	1.523 (9)
C1—C2	1.429 (9)	C8—H8	1.0000
C1—C6	1.452 (8)	C9—O2	1.426 (10)
C1—Fe1	2.039 (6)	C9—H9A	0.9900
C2—C3	1.407 (11)	C9—H9B	0.9900
C2—Fe1	2.048 (7)	C10—C11	1.398 (13)
C2—H2	0.9500	C10—C14	1.412 (12)
C3—C4	1.425 (11)	C10—Fe1	2.032 (7)
C3—Fe1	2.040 (11)	C10—H10	0.9500
C3—H3	0.9500	C11—C12	1.385 (15)
C4—C5	1.413 (9)	C11—Fe1	2.030 (9)
C4—Fe1	2.045 (8)	C11—H11	0.9500
C4—H4	0.9500	C12—C13	1.360 (14)
C5—Fe1	2.046 (6)	C12—Fe1	2.037 (12)
C5—H5	0.9500	C12—H12	0.9500
C6—N1	1.279 (7)	C13—C14	1.372 (12)
C6—O1	1.347 (7)	C13—Fe1	2.025 (9)
C7—O1	1.447 (7)	C13—H13	0.9500
C7—C8	1.533 (8)	C14—Fe1	2.029 (7)
C7—H7A	0.9900	C14—H14	0.9500
C7—H7B	0.9900	O2—H20	0.88 (7)
C8—N1	1.485 (8)		
C5—C1—C2	108.0 (5)	C11—C12—Fe1	69.8 (6)

C5—C1—C6	125.5 (5)	C13—C12—H12	126.7
C2—C1—C6	126.4 (6)	C11—C12—H12	126.7
C5—C1—Fe1	70.1 (3)	Fe1—C12—H12	125.2
C2—C1—Fe1	69.9 (4)	C12—C13—C14	111.0 (9)
C6—C1—Fe1	127.3 (5)	C12—C13—Fe1	70.9 (6)
C3—C2—C1	107.4 (6)	C14—C13—Fe1	70.4 (5)
C3—C2—Fe1	69.6 (5)	C12—C13—H13	124.5
C1—C2—Fe1	69.2 (4)	C14—C13—H13	124.5
C3—C2—H2	126.3	Fe1—C13—H13	125.8
C1—C2—H2	126.3	C13—C14—C10	106.8 (8)
Fe1—C2—H2	126.5	C13—C14—Fe1	70.1 (4)
C2—C3—C4	108.7 (7)	C10—C14—Fe1	69.8 (4)
C2—C3—Fe1	70.2 (5)	C13—C14—H14	126.6
C4—C3—Fe1	69.8 (5)	C10—C14—H14	126.6
C2—C3—H3	125.7	Fe1—C14—H14	125.2
C4—C3—H3	125.7	C13—Fe1—C11	65.8 (4)
Fe1—C3—H3	126.0	C13—Fe1—C14	39.6 (3)
C5—C4—C3	107.3 (6)	C11—Fe1—C14	67.3 (4)
C5—C4—Fe1	69.8 (4)	C13—Fe1—C10	66.8 (3)
C3—C4—Fe1	69.4 (5)	C11—Fe1—C10	40.3 (4)
C5—C4—H4	126.3	C14—Fe1—C10	40.7 (3)
C3—C4—H4	126.3	C13—Fe1—C12	39.1 (4)
Fe1—C4—H4	126.0	C11—Fe1—C12	39.8 (4)
C1—C5—C4	108.5 (6)	C14—Fe1—C12	67.2 (4)
C1—C5—Fe1	69.6 (3)	C10—Fe1—C12	67.8 (4)
C4—C5—Fe1	69.8 (4)	C13—Fe1—C1	156.0 (4)
C1—C5—H5	125.7	C11—Fe1—C1	108.8 (3)
C4—C5—H5	125.7	C14—Fe1—C1	162.7 (3)
Fe1—C5—H5	126.5	C10—Fe1—C1	125.4 (3)
N1—C6—O1	118.5 (5)	C12—Fe1—C1	121.4 (4)
N1—C6—C1	126.1 (5)	C13—Fe1—C3	125.9 (4)
O1—C6—C1	115.3 (5)	C11—Fe1—C3	158.1 (4)
O1—C7—C8	104.3 (5)	C14—Fe1—C3	108.8 (4)
O1—C7—H7A	110.9	C10—Fe1—C3	122.6 (4)
C8—C7—H7A	110.9	C12—Fe1—C3	160.6 (4)
O1—C7—H7B	110.9	C1—Fe1—C3	68.1 (3)
C8—C7—H7B	110.9	C13—Fe1—C5	121.6 (3)
H7A—C7—H7B	108.9	C11—Fe1—C5	124.6 (4)
N1—C8—C9	110.5 (5)	C14—Fe1—C5	156.0 (3)
N1—C8—C7	103.9 (5)	C10—Fe1—C5	161.3 (3)
C9—C8—C7	112.6 (6)	C12—Fe1—C5	107.4 (4)
N1—C8—H8	109.9	C1—Fe1—C5	40.3 (2)
C9—C8—H8	109.9	C3—Fe1—C5	68.0 (3)
C7—C8—H8	109.9	C13—Fe1—C4	108.4 (3)
O2—C9—C8	112.5 (5)	C11—Fe1—C4	160.1 (4)
O2—C9—H9A	109.1	C14—Fe1—C4	121.4 (3)
C8—C9—H9A	109.1	C10—Fe1—C4	157.4 (4)
O2—C9—H9B	109.1	C12—Fe1—C4	123.6 (4)

C8—C9—H9B	109.1	C1—Fe1—C4	68.2 (3)
H9A—C9—H9B	107.8	C3—Fe1—C4	40.8 (3)
C11—C10—C14	106.4 (7)	C5—Fe1—C4	40.4 (2)
C11—C10—Fe1	69.8 (5)	C13—Fe1—C2	162.0 (4)
C14—C10—Fe1	69.6 (4)	C11—Fe1—C2	123.2 (3)
C11—C10—H10	126.8	C14—Fe1—C2	125.8 (3)
C14—C10—H10	126.8	C10—Fe1—C2	108.9 (3)
Fe1—C10—H10	125.5	C12—Fe1—C2	157.5 (4)
C12—C11—C10	109.2 (9)	C1—Fe1—C2	40.9 (3)
C12—C11—Fe1	70.4 (6)	C3—Fe1—C2	40.2 (3)
C10—C11—Fe1	70.0 (5)	C5—Fe1—C2	68.2 (3)
C12—C11—H11	125.4	C4—Fe1—C2	68.4 (3)
C10—C11—H11	125.4	C6—N1—C8	106.4 (5)
Fe1—C11—H11	125.8	C6—O1—C7	106.2 (4)
C13—C12—C11	106.7 (10)	C9—O2—H20	116 (5)
C13—C12—Fe1	69.9 (6)		
C5—C1—C2—C3	-0.7 (8)	C13—C12—Fe1—C14	-36.0 (5)
C6—C1—C2—C3	-178.6 (7)	C11—C12—Fe1—C14	81.4 (6)
Fe1—C1—C2—C3	59.3 (5)	C13—C12—Fe1—C10	-80.2 (6)
C5—C1—C2—Fe1	-60.0 (4)	C11—C12—Fe1—C10	37.2 (6)
C6—C1—C2—Fe1	122.1 (7)	C13—C12—Fe1—C1	160.9 (5)
C1—C2—C3—C4	0.3 (9)	C11—C12—Fe1—C1	-81.7 (7)
Fe1—C2—C3—C4	59.4 (6)	C13—C12—Fe1—C3	45.9 (11)
C1—C2—C3—Fe1	-59.1 (5)	C11—C12—Fe1—C3	163.3 (8)
C2—C3—C4—C5	0.2 (9)	C13—C12—Fe1—C5	119.0 (6)
Fe1—C3—C4—C5	59.8 (5)	C11—C12—Fe1—C5	-123.6 (6)
C2—C3—C4—Fe1	-59.6 (6)	C13—C12—Fe1—C4	77.6 (7)
C2—C1—C5—C4	0.8 (7)	C11—C12—Fe1—C4	-165.1 (5)
C6—C1—C5—C4	178.7 (6)	C13—C12—Fe1—C2	-166.0 (7)
Fe1—C1—C5—C4	-59.0 (5)	C11—C12—Fe1—C2	-48.6 (12)
C2—C1—C5—Fe1	59.8 (4)	C5—C1—Fe1—C13	-49.2 (9)
C6—C1—C5—Fe1	-122.2 (7)	C2—C1—Fe1—C13	-168.1 (8)
C3—C4—C5—C1	-0.6 (8)	C6—C1—Fe1—C13	70.8 (10)
Fe1—C4—C5—C1	58.9 (4)	C5—C1—Fe1—C11	-121.8 (5)
C3—C4—C5—Fe1	-59.5 (5)	C2—C1—Fe1—C11	119.3 (5)
C5—C1—C6—N1	-7.2 (11)	C6—C1—Fe1—C11	-1.7 (7)
C2—C1—C6—N1	170.3 (7)	C5—C1—Fe1—C14	164.3 (12)
Fe1—C1—C6—N1	-98.3 (7)	C2—C1—Fe1—C14	45.4 (14)
C5—C1—C6—O1	176.1 (6)	C6—C1—Fe1—C14	-75.6 (14)
C2—C1—C6—O1	-6.3 (10)	C5—C1—Fe1—C10	-163.4 (5)
Fe1—C1—C6—O1	85.1 (7)	C2—C1—Fe1—C10	77.7 (6)
O1—C7—C8—N1	8.7 (6)	C6—C1—Fe1—C10	-43.4 (7)
O1—C7—C8—C9	-110.9 (6)	C5—C1—Fe1—C12	-79.7 (6)
N1—C8—C9—O2	-73.7 (7)	C2—C1—Fe1—C12	161.4 (6)
C7—C8—C9—O2	41.9 (7)	C6—C1—Fe1—C12	40.3 (7)
C14—C10—C11—C12	-0.6 (10)	C5—C1—Fe1—C3	81.3 (4)
Fe1—C10—C11—C12	59.7 (7)	C2—C1—Fe1—C3	-37.6 (4)

C14—C10—C11—Fe1	-60.2 (5)	C6—C1—Fe1—C3	-158.6 (6)
C10—C11—C12—C13	1.1 (11)	C2—C1—Fe1—C5	-118.9 (5)
Fe1—C11—C12—C13	60.6 (7)	C6—C1—Fe1—C5	120.1 (7)
C10—C11—C12—Fe1	-59.4 (6)	C5—C1—Fe1—C4	37.2 (4)
C11—C12—C13—C14	-1.3 (11)	C2—C1—Fe1—C4	-81.7 (4)
Fe1—C12—C13—C14	59.1 (7)	C6—C1—Fe1—C4	157.3 (6)
C11—C12—C13—Fe1	-60.5 (7)	C5—C1—Fe1—C2	118.9 (5)
C12—C13—C14—C10	1.0 (10)	C6—C1—Fe1—C2	-121.0 (7)
Fe1—C13—C14—C10	60.4 (5)	C2—C3—Fe1—C13	-164.3 (4)
C12—C13—C14—Fe1	-59.4 (7)	C4—C3—Fe1—C13	76.0 (6)
C11—C10—C14—C13	-0.2 (9)	C2—C3—Fe1—C11	-48.0 (12)
Fe1—C10—C14—C13	-60.6 (6)	C4—C3—Fe1—C11	-167.7 (8)
C11—C10—C14—Fe1	60.4 (5)	C2—C3—Fe1—C14	-123.7 (5)
C12—C13—Fe1—C11	38.6 (6)	C4—C3—Fe1—C14	116.6 (5)
C14—C13—Fe1—C11	-83.1 (6)	C2—C3—Fe1—C10	-80.8 (6)
C12—C13—Fe1—C14	121.7 (9)	C4—C3—Fe1—C10	159.5 (4)
C12—C13—Fe1—C10	82.7 (7)	C2—C3—Fe1—C12	161.7 (9)
C14—C13—Fe1—C10	-39.0 (5)	C4—C3—Fe1—C12	42.0 (10)
C14—C13—Fe1—C12	-121.7 (9)	C2—C3—Fe1—C1	38.2 (4)
C12—C13—Fe1—C1	-43.3 (11)	C4—C3—Fe1—C1	-81.5 (5)
C14—C13—Fe1—C1	-165.0 (7)	C2—C3—Fe1—C5	81.8 (5)
C12—C13—Fe1—C3	-162.9 (5)	C4—C3—Fe1—C5	-37.9 (4)
C14—C13—Fe1—C3	75.4 (7)	C2—C3—Fe1—C4	119.7 (7)
C12—C13—Fe1—C5	-78.5 (7)	C4—C3—Fe1—C2	-119.7 (7)
C14—C13—Fe1—C5	159.8 (5)	C1—C5—Fe1—C13	158.8 (5)
C12—C13—Fe1—C4	-120.9 (7)	C4—C5—Fe1—C13	-81.3 (6)
C14—C13—Fe1—C4	117.3 (6)	C1—C5—Fe1—C11	78.0 (5)
C12—C13—Fe1—C2	162.5 (10)	C4—C5—Fe1—C11	-162.1 (5)
C14—C13—Fe1—C2	40.8 (13)	C1—C5—Fe1—C14	-168.6 (9)
C12—C11—Fe1—C13	-37.9 (6)	C4—C5—Fe1—C14	-48.7 (10)
C10—C11—Fe1—C13	82.1 (5)	C1—C5—Fe1—C10	46.5 (12)
C12—C11—Fe1—C14	-81.2 (7)	C4—C5—Fe1—C10	166.5 (11)
C10—C11—Fe1—C14	38.9 (5)	C1—C5—Fe1—C12	118.4 (6)
C12—C11—Fe1—C10	-120.1 (8)	C4—C5—Fe1—C12	-121.7 (6)
C10—C11—Fe1—C12	120.1 (8)	C4—C5—Fe1—C1	119.9 (6)
C12—C11—Fe1—C1	116.9 (6)	C1—C5—Fe1—C3	-81.7 (4)
C10—C11—Fe1—C1	-123.1 (5)	C4—C5—Fe1—C3	38.3 (4)
C12—C11—Fe1—C3	-165.1 (8)	C1—C5—Fe1—C4	-119.9 (6)
C10—C11—Fe1—C3	-45.1 (12)	C1—C5—Fe1—C2	-38.1 (4)
C12—C11—Fe1—C5	74.9 (7)	C4—C5—Fe1—C2	81.8 (4)
C10—C11—Fe1—C5	-165.0 (4)	C5—C4—Fe1—C13	117.5 (5)
C12—C11—Fe1—C4	39.1 (12)	C3—C4—Fe1—C13	-124.0 (6)
C10—C11—Fe1—C4	159.1 (8)	C5—C4—Fe1—C11	48.0 (11)
C12—C11—Fe1—C2	159.9 (6)	C3—C4—Fe1—C11	166.5 (9)
C10—C11—Fe1—C2	-80.0 (6)	C5—C4—Fe1—C14	159.0 (5)
C10—C14—Fe1—C13	-117.4 (8)	C3—C4—Fe1—C14	-82.5 (6)
C13—C14—Fe1—C11	78.9 (6)	C5—C4—Fe1—C10	-168.8 (8)
C10—C14—Fe1—C11	-38.5 (5)	C3—C4—Fe1—C10	-50.3 (10)

C13—C14—Fe1—C10	117.4 (8)	C5—C4—Fe1—C12	77.0 (6)
C13—C14—Fe1—C12	35.6 (6)	C3—C4—Fe1—C12	-164.5 (5)
C10—C14—Fe1—C12	-81.8 (6)	C5—C4—Fe1—C1	-37.2 (4)
C13—C14—Fe1—C1	159.3 (12)	C3—C4—Fe1—C1	81.3 (5)
C10—C14—Fe1—C1	41.9 (14)	C5—C4—Fe1—C3	-118.5 (6)
C13—C14—Fe1—C3	-124.1 (6)	C3—C4—Fe1—C5	118.5 (6)
C10—C14—Fe1—C3	118.5 (6)	C5—C4—Fe1—C2	-81.4 (4)
C13—C14—Fe1—C5	-46.1 (11)	C3—C4—Fe1—C2	37.1 (4)
C10—C14—Fe1—C5	-163.6 (9)	C3—C2—Fe1—C13	45.4 (12)
C13—C14—Fe1—C4	-80.9 (7)	C1—C2—Fe1—C13	164.3 (9)
C10—C14—Fe1—C4	161.7 (5)	C3—C2—Fe1—C11	160.7 (6)
C13—C14—Fe1—C2	-165.6 (6)	C1—C2—Fe1—C11	-80.4 (5)
C10—C14—Fe1—C2	77.0 (6)	C3—C2—Fe1—C14	76.3 (6)
C11—C10—Fe1—C13	-79.3 (6)	C1—C2—Fe1—C14	-164.9 (4)
C14—C10—Fe1—C13	37.9 (5)	C3—C2—Fe1—C10	118.4 (6)
C14—C10—Fe1—C11	117.3 (7)	C1—C2—Fe1—C10	-122.7 (5)
C11—C10—Fe1—C14	-117.3 (7)	C3—C2—Fe1—C12	-164.2 (8)
C11—C10—Fe1—C12	-36.8 (6)	C1—C2—Fe1—C12	-45.3 (11)
C14—C10—Fe1—C12	80.5 (6)	C3—C2—Fe1—C1	-118.9 (6)
C11—C10—Fe1—C1	76.8 (6)	C1—C2—Fe1—C3	118.9 (6)
C14—C10—Fe1—C1	-165.9 (5)	C3—C2—Fe1—C5	-81.3 (5)
C11—C10—Fe1—C3	161.8 (5)	C1—C2—Fe1—C5	37.6 (4)
C14—C10—Fe1—C3	-80.9 (6)	C3—C2—Fe1—C4	-37.6 (5)
C11—C10—Fe1—C5	41.6 (13)	C1—C2—Fe1—C4	81.3 (4)
C14—C10—Fe1—C5	158.9 (10)	O1—C6—N1—C8	3.2 (7)
C11—C10—Fe1—C4	-161.6 (8)	C1—C6—N1—C8	-173.4 (7)
C14—C10—Fe1—C4	-44.3 (10)	C9—C8—N1—C6	113.6 (6)
C11—C10—Fe1—C2	119.4 (5)	C7—C8—N1—C6	-7.3 (6)
C14—C10—Fe1—C2	-123.3 (5)	N1—C6—O1—C7	2.7 (8)
C11—C12—Fe1—C13	117.4 (9)	C1—C6—O1—C7	179.7 (6)
C13—C12—Fe1—C11	-117.4 (9)	C8—C7—O1—C6	-7.1 (7)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O2—H20...N1 ⁱ	0.87 (7)	2.02 (8)	2.877 (7)	165 (7)

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