

2-Ferrocenyl-6-methylpyridin-3-ol

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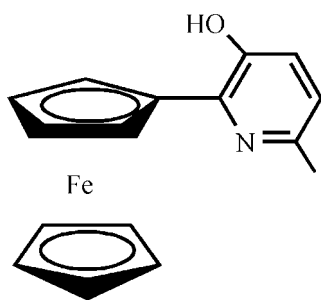
Received 16 November 2008; accepted 24 November 2008

Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; disorder in main residue; R factor = 0.037; wR factor = 0.099; data-to-parameter ratio = 14.0.

In the title compound, $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{11}\text{H}_{10}\text{NO})]$, the dihedral angle between the pyridyl and substituted cyclopentadienyl rings is $20.4(3)^\circ$. The H atoms of the methyl group are disordered over two positions; their site-occupation factors were fixed at 0.5. The crystal structure is stabilized by well defined intermolecular $\text{O}-\text{H}\cdots\text{N}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, leading to the formation of a two-dimensional network parallel to (101).

Related literature

For ferrocene and its derivatives, see: Beletskaya *et al.* (2001); Hayashi & Togni (1995); Kealy & Pauson (1951); Sarhan & Izumi (2003); Staveren & Metzler-Nolte (2004); Xu *et al.* (2007).



Experimental

Crystal data

$[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{11}\text{H}_{10}\text{NO})]$
 $M_r = 293.14$

Monoclinic, $P2_1/n$
 $a = 10.4370(13)$ Å
 $b = 12.7196(15)$ Å
 $c = 10.5424(13)$ Å
 $\beta = 111.0330(10)^\circ$

$V = 1306.3(3)$ Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 1.14$ mm⁻¹
 $T = 291(2)$ K
 $0.37 \times 0.23 \times 0.21$ mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.675$, $T_{\max} = 0.793$

7569 measured reflections
2422 independent reflections
1970 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.099$
 $S = 1.08$
2422 reflections

173 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.63$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.54$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{N1}^i$	0.82	1.96	2.774 (3)	169
$\text{C7}-\text{H7}\cdots\text{O1}$	0.98	2.39	2.866 (4)	109

Symmetry code: (i) $x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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*.

This work was supported by the Doctoral Foundation of Luoyang Normal University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2173).

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supplementary materials

Acta Cryst. (2008). E64, m1633 [doi:10.1107/S1600536808039597]

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Comment

Since the discovery of ferrocene in the 1950's (Kealy & Pauson, 1951), the fascinating structural properties of ferrocene and its derivatives have been the subject of increasing interest in all fields of organometallic chemistry (Hayashi *et al.*, 1995; Staveren *et al.*, 2004; Xu *et al.*, 2007). Among them, ferrocene-heterocycles are one of the most important ones (Sarhan & Izumi, 2003). Herein we report the crystal structure of the title compound.

A view of the molecular structure of the title compound is given in Fig.1. The hydrogen atoms of methyl groups are disordered; site-occupation factors were fixed at 0.5. The pyridyl and Cp ring form a dihedral angle of $20.4(3)^\circ$. In the crystal of the title compound, intermolecular O—H \cdots N and C—H \cdots O hydrogen bonds are present (Table 1), resulting in a two-dimensional supramolecular architecture (Fig.2).

Experimental

The title compound was prepared as described in literature (Beletskaya *et al.*, 2001) and recrystallized from dichloromethane-petroleum ether solution at room temperature to give the desired product as red crystals suitable for single-crystal X-ray diffraction.

Refinement

H atoms attached to C atoms of the title compound were placed in geometrically idealized positions and treated as riding with C—H distances constrained to 0.93–0.96 Å, and with $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})(1.5U_{\text{eq}} \text{ for methyl H})$.

Figures

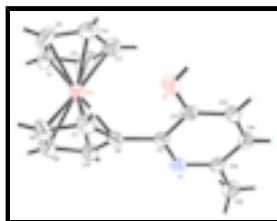


Fig. 1. The molecular structure of the title compound with displacement ellipsoids at the 30% probability level. Only one disordered component of the methyl group is shown.

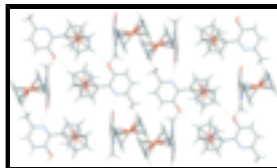


Fig. 2. Partial view of the crystal packing showing the intermolecular O—H \cdots N and C—H \cdots O hydrogen bonds. One disordered component of the methyl group has been omitted for clarity.

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Crystal data

[Fe(C₅H₅)(C₁₁H₁₀NO)]

$M_r = 293.14$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 10.4370$ (13) Å

$b = 12.7196$ (15) Å

$c = 10.5424$ (13) Å

$\beta = 111.0330$ (10)°

$V = 1306.3$ (3) Å³

$Z = 4$

$F_{000} = 608$

$D_x = 1.491$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 2766 reflections

$\theta = 2.4$ – 25.0 °

$\mu = 1.14$ mm⁻¹

$T = 291$ (2) K

Block, red

$0.37 \times 0.23 \times 0.21$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 291$ (2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.675$, $T_{\max} = 0.794$

7569 measured reflections

2422 independent reflections

1970 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.021$

$\theta_{\text{max}} = 25.5$ °

$\theta_{\text{min}} = 2.4$ °

$h = -10 \rightarrow 12$

$k = -15 \rightarrow 15$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.037$

$wR(F^2) = 0.099$

$S = 1.09$

2422 reflections

173 parameters

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

$$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 0.7167P]$$

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

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

$\Delta\rho_{\text{max}} = 0.63$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.54$ e Å⁻³

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 $F^2 > \sigma(F^2)$ 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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Fe1	0.35569 (4)	1.02041 (3)	0.20685 (4)	0.04595 (16)	
O1	0.5672 (2)	0.78281 (18)	0.36235 (18)	0.0576 (5)	
H1	0.6489	0.7688	0.3993	0.086*	
N1	0.3444 (2)	0.74252 (16)	0.0124 (2)	0.0424 (5)	
C1	0.3813 (5)	1.1764 (3)	0.1792 (5)	0.0962 (14)	
H1A	0.3075	1.2283	0.1454	0.115*	
C2	0.4350 (5)	1.1151 (3)	0.0982 (4)	0.0905 (13)	
H2	0.4057	1.1177	-0.0011	0.109*	
C3	0.5377 (4)	1.0523 (3)	0.1836 (4)	0.0788 (11)	
H3	0.5932	1.0019	0.1552	0.095*	
C4	0.5481 (4)	1.0718 (3)	0.3185 (4)	0.0827 (11)	
H4	0.6125	1.0386	0.4004	0.099*	
C5	0.4490 (4)	1.1502 (3)	0.3136 (4)	0.0856 (12)	
H5	0.4325	1.1806	0.3918	0.103*	
C6	0.3115 (3)	0.8626 (2)	0.1744 (3)	0.0452 (6)	
C7	0.3146 (3)	0.8949 (3)	0.3049 (3)	0.0573 (7)	
H7	0.3754	0.8666	0.3922	0.069*	
C8	0.2150 (3)	0.9752 (3)	0.2872 (4)	0.0693 (9)	
H8	0.1948	1.0114	0.3600	0.083*	
C9	0.1511 (3)	0.9943 (3)	0.1476 (4)	0.0778 (11)	
H9	0.0787	1.0462	0.1061	0.093*	
C10	0.2095 (3)	0.9257 (3)	0.0766 (3)	0.0638 (9)	
H10	0.1849	0.9227	-0.0222	0.077*	
C11	0.3946 (2)	0.78116 (19)	0.1409 (2)	0.0389 (6)	

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C12	0.5209 (3)	0.7445 (2)	0.2335 (2)	0.0419 (6)	
C13	0.5943 (3)	0.6722 (2)	0.1894 (3)	0.0487 (7)	
H13	0.6780	0.6472	0.2490	0.058*	
C14	0.5436 (3)	0.6372 (2)	0.0573 (3)	0.0489 (6)	
H14	0.5936	0.5896	0.0264	0.059*	
C15	0.4175 (3)	0.6734 (2)	-0.0295 (3)	0.0455 (6)	
C16	0.3599 (3)	0.6378 (3)	-0.1758 (3)	0.0637 (8)	
H16A	0.2724	0.6705	-0.2207	0.096*	0.50
H16B	0.3490	0.5628	-0.1790	0.096*	0.50
H16C	0.4217	0.6574	-0.2206	0.096*	0.50
H16D	0.4230	0.5900	-0.1929	0.096*	0.50
H16E	0.3464	0.6977	-0.2345	0.096*	0.50
H16F	0.2737	0.6030	-0.1929	0.096*	0.50

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0494 (3)	0.0480 (3)	0.0396 (2)	0.00711 (17)	0.01483 (18)	-0.00218 (16)
O1	0.0420 (11)	0.0758 (14)	0.0404 (10)	0.0147 (10)	-0.0031 (8)	-0.0069 (9)
N1	0.0351 (11)	0.0414 (12)	0.0407 (11)	-0.0034 (9)	0.0014 (9)	0.0023 (9)
C1	0.143 (4)	0.044 (2)	0.120 (4)	0.011 (2)	0.070 (3)	-0.003 (2)
C2	0.150 (4)	0.059 (2)	0.088 (3)	-0.012 (2)	0.074 (3)	-0.002 (2)
C3	0.080 (3)	0.067 (2)	0.110 (3)	-0.024 (2)	0.058 (2)	-0.031 (2)
C4	0.063 (2)	0.089 (3)	0.092 (3)	-0.021 (2)	0.022 (2)	-0.033 (2)
C5	0.102 (3)	0.076 (2)	0.091 (3)	-0.020 (2)	0.050 (2)	-0.039 (2)
C6	0.0298 (13)	0.0498 (16)	0.0499 (15)	-0.0026 (11)	0.0069 (11)	0.0015 (12)
C7	0.0532 (18)	0.068 (2)	0.0575 (17)	0.0024 (15)	0.0282 (14)	0.0088 (14)
C8	0.0517 (19)	0.085 (2)	0.084 (2)	0.0068 (17)	0.0393 (19)	-0.0064 (18)
C9	0.0382 (17)	0.090 (3)	0.089 (3)	0.0194 (17)	0.0033 (18)	-0.013 (2)
C10	0.0414 (16)	0.071 (2)	0.0606 (18)	0.0121 (15)	-0.0037 (14)	-0.0132 (16)
C11	0.0315 (13)	0.0380 (13)	0.0413 (13)	-0.0045 (10)	0.0060 (11)	0.0036 (10)
C12	0.0370 (14)	0.0419 (14)	0.0375 (13)	-0.0012 (11)	0.0019 (11)	0.0020 (10)
C13	0.0405 (15)	0.0439 (15)	0.0489 (15)	0.0084 (12)	0.0003 (12)	0.0034 (12)
C14	0.0488 (16)	0.0385 (14)	0.0525 (15)	0.0045 (12)	0.0097 (13)	-0.0019 (11)
C15	0.0464 (16)	0.0372 (14)	0.0450 (14)	-0.0056 (12)	0.0067 (12)	-0.0005 (11)
C16	0.063 (2)	0.0625 (19)	0.0502 (17)	0.0023 (16)	0.0019 (15)	-0.0102 (14)

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

Fe1—C8	2.024 (3)	C6—C7	1.426 (4)
Fe1—C9	2.025 (3)	C6—C10	1.433 (4)
Fe1—C7	2.029 (3)	C6—C11	1.473 (4)
Fe1—C2	2.032 (4)	C7—C8	1.421 (4)
Fe1—C4	2.036 (3)	C7—H7	0.9800
Fe1—C1	2.036 (4)	C8—C9	1.401 (5)
Fe1—C5	2.038 (4)	C8—H8	0.9800
Fe1—C10	2.040 (3)	C9—C10	1.421 (5)
Fe1—C3	2.041 (4)	C9—H9	0.9800
Fe1—C6	2.061 (3)	C10—H10	0.9800

O1—C12	1.358 (3)	C11—C12	1.408 (3)
O1—H1	0.8200	C12—C13	1.381 (4)
N1—C15	1.339 (3)	C13—C14	1.374 (4)
N1—C11	1.357 (3)	C13—H13	0.9300
C1—C5	1.377 (6)	C14—C15	1.385 (4)
C1—C2	1.412 (5)	C14—H14	0.9300
C1—H1A	0.9800	C15—C16	1.509 (4)
C2—C3	1.381 (6)	C16—H16A	0.9600
C2—H2	0.9800	C16—H16B	0.9600
C3—C4	1.408 (5)	C16—H16C	0.9600
C3—H3	0.9800	C16—H16D	0.9600
C4—C5	1.425 (6)	C16—H16E	0.9600
C4—H4	0.9800	C16—H16F	0.9600
C5—H5	0.9800		
C8—Fe1—C9	40.49 (16)	C1—C5—Fe1	70.2 (2)
C8—Fe1—C7	41.06 (13)	C4—C5—Fe1	69.5 (2)
C9—Fe1—C7	68.66 (15)	C1—C5—H5	126.2
C8—Fe1—C2	155.18 (17)	C4—C5—H5	126.2
C9—Fe1—C2	121.4 (2)	Fe1—C5—H5	126.2
C7—Fe1—C2	163.08 (15)	C7—C6—C10	106.6 (3)
C8—Fe1—C4	124.23 (16)	C7—C6—C11	128.5 (2)
C9—Fe1—C4	160.47 (16)	C10—C6—C11	124.9 (3)
C7—Fe1—C4	107.62 (16)	C7—C6—Fe1	68.41 (17)
C2—Fe1—C4	67.60 (19)	C10—C6—Fe1	68.77 (17)
C8—Fe1—C1	119.26 (17)	C11—C6—Fe1	127.50 (18)
C9—Fe1—C1	107.08 (18)	C8—C7—C6	108.5 (3)
C7—Fe1—C1	154.37 (15)	C8—C7—Fe1	69.29 (19)
C2—Fe1—C1	40.61 (16)	C6—C7—Fe1	70.80 (16)
C4—Fe1—C1	67.5 (2)	C8—C7—H7	125.7
C8—Fe1—C5	105.90 (16)	C6—C7—H7	125.7
C9—Fe1—C5	123.03 (16)	Fe1—C7—H7	125.7
C7—Fe1—C5	120.16 (16)	C9—C8—C7	108.2 (3)
C2—Fe1—C5	67.68 (17)	C9—C8—Fe1	69.8 (2)
C4—Fe1—C5	40.93 (16)	C7—C8—Fe1	69.66 (17)
C1—Fe1—C5	39.52 (16)	C9—C8—H8	125.9
C8—Fe1—C10	68.53 (15)	C7—C8—H8	125.9
C9—Fe1—C10	40.92 (14)	Fe1—C8—H8	125.9
C7—Fe1—C10	68.58 (14)	C8—C9—C10	108.3 (3)
C2—Fe1—C10	109.16 (17)	C8—C9—Fe1	69.71 (19)
C4—Fe1—C10	157.32 (14)	C10—C9—Fe1	70.09 (18)
C1—Fe1—C10	125.72 (18)	C8—C9—H9	125.8
C5—Fe1—C10	160.69 (16)	C10—C9—H9	125.8
C8—Fe1—C3	162.32 (18)	Fe1—C9—H9	125.8
C9—Fe1—C3	156.78 (18)	C9—C10—C6	108.3 (3)
C7—Fe1—C3	126.37 (16)	C9—C10—Fe1	68.99 (19)
C2—Fe1—C3	39.63 (17)	C6—C10—Fe1	70.33 (16)
C4—Fe1—C3	40.41 (15)	C9—C10—H10	125.9
C1—Fe1—C3	67.29 (18)	C6—C10—H10	125.9
C5—Fe1—C3	67.95 (15)	Fe1—C10—H10	125.9

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C10—Fe1—C3	122.69 (14)	N1—C11—C12	120.2 (2)
C8—Fe1—C6	68.91 (13)	N1—C11—C6	116.3 (2)
C9—Fe1—C6	68.94 (13)	C12—C11—C6	123.5 (2)
C7—Fe1—C6	40.79 (11)	O1—C12—C13	122.3 (2)
C2—Fe1—C6	126.58 (13)	O1—C12—C11	118.9 (2)
C4—Fe1—C6	121.60 (15)	C13—C12—C11	118.8 (2)
C1—Fe1—C6	163.36 (16)	C14—C13—C12	119.9 (2)
C5—Fe1—C6	156.22 (16)	C14—C13—H13	120.0
C10—Fe1—C6	40.90 (11)	C12—C13—H13	120.0
C3—Fe1—C6	109.62 (13)	C13—C14—C15	119.4 (3)
C12—O1—H1	109.5	C13—C14—H14	120.3
C15—N1—C11	120.4 (2)	C15—C14—H14	120.3
C5—C1—C2	108.7 (4)	N1—C15—C14	121.3 (2)
C5—C1—Fe1	70.3 (2)	N1—C15—C16	118.0 (2)
C2—C1—Fe1	69.5 (2)	C14—C15—C16	120.7 (3)
C5—C1—H1A	125.7	C15—C16—H16A	109.5
C2—C1—H1A	125.7	C15—C16—H16B	109.5
Fe1—C1—H1A	125.7	H16A—C16—H16B	109.5
C3—C2—C1	108.0 (4)	C15—C16—H16C	109.5
C3—C2—Fe1	70.5 (2)	H16A—C16—H16C	109.5
C1—C2—Fe1	69.9 (2)	H16B—C16—H16C	109.5
C3—C2—H2	126.0	C15—C16—H16D	109.5
C1—C2—H2	126.0	H16A—C16—H16D	141.1
Fe1—C2—H2	126.0	H16B—C16—H16D	56.3
C2—C3—C4	108.5 (4)	H16C—C16—H16D	56.3
C2—C3—Fe1	69.8 (2)	C15—C16—H16E	109.5
C4—C3—Fe1	69.6 (2)	H16A—C16—H16E	56.3
C2—C3—H3	125.8	H16B—C16—H16E	141.1
C4—C3—H3	125.8	H16C—C16—H16E	56.3
Fe1—C3—H3	125.8	H16D—C16—H16E	109.5
C3—C4—C5	107.2 (4)	C15—C16—H16F	109.5
C3—C4—Fe1	70.0 (2)	H16A—C16—H16F	56.3
C5—C4—Fe1	69.6 (2)	H16B—C16—H16F	56.3
C3—C4—H4	126.4	H16C—C16—H16F	141.1
C5—C4—H4	126.4	H16D—C16—H16F	109.5
Fe1—C4—H4	126.4	H16E—C16—H16F	109.5
C1—C5—C4	107.7 (3)		
C8—Fe1—C1—C5	79.3 (3)	C8—Fe1—C6—C11	-160.5 (3)
C9—Fe1—C1—C5	121.6 (3)	C9—Fe1—C6—C11	155.9 (3)
C7—Fe1—C1—C5	45.4 (5)	C7—Fe1—C6—C11	-122.7 (3)
C2—Fe1—C1—C5	-119.8 (4)	C2—Fe1—C6—C11	41.8 (3)
C4—Fe1—C1—C5	-38.5 (2)	C4—Fe1—C6—C11	-42.4 (3)
C10—Fe1—C1—C5	162.7 (2)	C1—Fe1—C6—C11	76.9 (6)
C3—Fe1—C1—C5	-82.4 (3)	C5—Fe1—C6—C11	-79.0 (4)
C6—Fe1—C1—C5	-165.0 (4)	C10—Fe1—C6—C11	118.3 (3)
C8—Fe1—C1—C2	-160.9 (3)	C3—Fe1—C6—C11	0.7 (3)
C9—Fe1—C1—C2	-118.6 (3)	C10—C6—C7—C8	0.8 (3)
C7—Fe1—C1—C2	165.3 (3)	C11—C6—C7—C8	-179.3 (3)
C4—Fe1—C1—C2	81.3 (3)	Fe1—C6—C7—C8	59.2 (2)

C5—Fe1—C1—C2	119.8 (4)	C10—C6—C7—Fe1	-58.4 (2)
C10—Fe1—C1—C2	-77.4 (3)	C11—C6—C7—Fe1	121.5 (3)
C3—Fe1—C1—C2	37.4 (3)	C9—Fe1—C7—C8	-37.4 (2)
C6—Fe1—C1—C2	-45.2 (7)	C2—Fe1—C7—C8	-167.0 (5)
C5—C1—C2—C3	-0.9 (5)	C4—Fe1—C7—C8	122.3 (2)
Fe1—C1—C2—C3	-60.5 (3)	C1—Fe1—C7—C8	47.7 (5)
C5—C1—C2—Fe1	59.6 (3)	C5—Fe1—C7—C8	79.3 (3)
C8—Fe1—C2—C3	161.4 (3)	C10—Fe1—C7—C8	-81.5 (2)
C9—Fe1—C2—C3	-162.0 (2)	C3—Fe1—C7—C8	163.0 (2)
C7—Fe1—C2—C3	-39.2 (6)	C6—Fe1—C7—C8	-119.5 (3)
C4—Fe1—C2—C3	37.5 (2)	C8—Fe1—C7—C6	119.5 (3)
C1—Fe1—C2—C3	118.6 (4)	C9—Fe1—C7—C6	82.08 (19)
C5—Fe1—C2—C3	81.9 (3)	C2—Fe1—C7—C6	-47.5 (6)
C10—Fe1—C2—C3	-118.5 (2)	C4—Fe1—C7—C6	-118.27 (18)
C6—Fe1—C2—C3	-76.1 (3)	C1—Fe1—C7—C6	167.2 (4)
C8—Fe1—C2—C1	42.8 (5)	C5—Fe1—C7—C6	-161.19 (19)
C9—Fe1—C2—C1	79.4 (3)	C10—Fe1—C7—C6	37.99 (17)
C7—Fe1—C2—C1	-157.8 (5)	C3—Fe1—C7—C6	-77.6 (2)
C4—Fe1—C2—C1	-81.1 (3)	C6—C7—C8—C9	-0.8 (4)
C5—Fe1—C2—C1	-36.6 (3)	Fe1—C7—C8—C9	59.4 (3)
C10—Fe1—C2—C1	123.0 (3)	C6—C7—C8—Fe1	-60.1 (2)
C3—Fe1—C2—C1	-118.6 (4)	C7—Fe1—C8—C9	-119.4 (3)
C6—Fe1—C2—C1	165.4 (3)	C2—Fe1—C8—C9	51.6 (5)
C1—C2—C3—C4	1.0 (5)	C4—Fe1—C8—C9	163.5 (2)
Fe1—C2—C3—C4	-59.1 (3)	C1—Fe1—C8—C9	82.1 (3)
C1—C2—C3—Fe1	60.1 (3)	C5—Fe1—C8—C9	122.6 (2)
C8—Fe1—C3—C2	-153.9 (4)	C10—Fe1—C8—C9	-37.8 (2)
C9—Fe1—C3—C2	42.0 (5)	C3—Fe1—C8—C9	-170.4 (4)
C7—Fe1—C3—C2	166.8 (2)	C6—Fe1—C8—C9	-81.9 (2)
C4—Fe1—C3—C2	-119.8 (3)	C9—Fe1—C8—C7	119.4 (3)
C1—Fe1—C3—C2	-38.3 (2)	C2—Fe1—C8—C7	171.0 (3)
C5—Fe1—C3—C2	-81.2 (3)	C4—Fe1—C8—C7	-77.1 (3)
C10—Fe1—C3—C2	80.6 (3)	C1—Fe1—C8—C7	-158.5 (2)
C6—Fe1—C3—C2	124.2 (2)	C5—Fe1—C8—C7	-117.9 (2)
C8—Fe1—C3—C4	-34.1 (6)	C10—Fe1—C8—C7	81.6 (2)
C9—Fe1—C3—C4	161.8 (4)	C3—Fe1—C8—C7	-51.0 (6)
C7—Fe1—C3—C4	-73.4 (3)	C6—Fe1—C8—C7	37.56 (19)
C2—Fe1—C3—C4	119.8 (3)	C7—C8—C9—C10	0.4 (4)
C1—Fe1—C3—C4	81.5 (3)	Fe1—C8—C9—C10	59.7 (3)
C5—Fe1—C3—C4	38.6 (3)	C7—C8—C9—Fe1	-59.3 (2)
C10—Fe1—C3—C4	-159.6 (2)	C7—Fe1—C9—C8	37.9 (2)
C6—Fe1—C3—C4	-116.1 (2)	C2—Fe1—C9—C8	-157.3 (2)
C2—C3—C4—C5	-0.7 (4)	C4—Fe1—C9—C8	-44.7 (6)
Fe1—C3—C4—C5	-59.9 (3)	C1—Fe1—C9—C8	-115.3 (2)
C2—C3—C4—Fe1	59.2 (3)	C5—Fe1—C9—C8	-75.0 (3)
C8—Fe1—C4—C3	168.1 (2)	C10—Fe1—C9—C8	119.4 (3)
C9—Fe1—C4—C3	-158.4 (5)	C3—Fe1—C9—C8	172.7 (3)
C7—Fe1—C4—C3	125.9 (3)	C6—Fe1—C9—C8	81.8 (2)
C2—Fe1—C4—C3	-36.8 (2)	C8—Fe1—C9—C10	-119.4 (3)

supplementary materials

C1—Fe1—C4—C3	-80.9 (3)	C7—Fe1—C9—C10	-81.5 (2)
C5—Fe1—C4—C3	-118.1 (4)	C2—Fe1—C9—C10	83.3 (3)
C10—Fe1—C4—C3	49.4 (5)	C4—Fe1—C9—C10	-164.1 (5)
C6—Fe1—C4—C3	83.4 (3)	C1—Fe1—C9—C10	125.3 (2)
C8—Fe1—C4—C5	-73.8 (3)	C5—Fe1—C9—C10	165.6 (2)
C9—Fe1—C4—C5	-40.3 (6)	C3—Fe1—C9—C10	53.3 (5)
C7—Fe1—C4—C5	-116.0 (3)	C6—Fe1—C9—C10	-37.6 (2)
C2—Fe1—C4—C5	81.3 (3)	C8—C9—C10—C6	0.1 (4)
C1—Fe1—C4—C5	37.2 (2)	Fe1—C9—C10—C6	59.6 (2)
C10—Fe1—C4—C5	167.5 (4)	C8—C9—C10—Fe1	-59.4 (3)
C3—Fe1—C4—C5	118.1 (4)	C7—C6—C10—C9	-0.6 (4)
C6—Fe1—C4—C5	-158.5 (2)	C11—C6—C10—C9	179.6 (3)
C2—C1—C5—C4	0.5 (5)	Fe1—C6—C10—C9	-58.7 (2)
Fe1—C1—C5—C4	59.6 (3)	C7—C6—C10—Fe1	58.1 (2)
C2—C1—C5—Fe1	-59.1 (3)	C11—C6—C10—Fe1	-121.7 (3)
C3—C4—C5—C1	0.2 (5)	C8—Fe1—C10—C9	37.4 (2)
Fe1—C4—C5—C1	-60.0 (3)	C7—Fe1—C10—C9	81.7 (2)
C3—C4—C5—Fe1	60.2 (2)	C2—Fe1—C10—C9	-116.2 (3)
C8—Fe1—C5—C1	-117.0 (3)	C4—Fe1—C10—C9	166.2 (4)
C9—Fe1—C5—C1	-76.2 (3)	C1—Fe1—C10—C9	-73.9 (3)
C7—Fe1—C5—C1	-159.1 (2)	C5—Fe1—C10—C9	-39.1 (6)
C2—Fe1—C5—C1	37.6 (3)	C3—Fe1—C10—C9	-157.9 (3)
C4—Fe1—C5—C1	118.7 (4)	C6—Fe1—C10—C9	119.6 (3)
C10—Fe1—C5—C1	-46.7 (6)	C8—Fe1—C10—C6	-82.2 (2)
C3—Fe1—C5—C1	80.6 (3)	C9—Fe1—C10—C6	-119.6 (3)
C6—Fe1—C5—C1	169.4 (3)	C7—Fe1—C10—C6	-37.89 (17)
C8—Fe1—C5—C4	124.4 (3)	C2—Fe1—C10—C6	124.2 (2)
C9—Fe1—C5—C4	165.1 (2)	C4—Fe1—C10—C6	46.6 (5)
C7—Fe1—C5—C4	82.2 (3)	C1—Fe1—C10—C6	166.5 (2)
C2—Fe1—C5—C4	-81.1 (3)	C5—Fe1—C10—C6	-158.7 (4)
C1—Fe1—C5—C4	-118.7 (4)	C3—Fe1—C10—C6	82.4 (2)
C10—Fe1—C5—C4	-165.4 (4)	C15—N1—C11—C12	-3.4 (4)
C3—Fe1—C5—C4	-38.1 (3)	C15—N1—C11—C6	175.6 (2)
C6—Fe1—C5—C4	50.7 (4)	C7—C6—C11—N1	160.0 (3)
C8—Fe1—C6—C7	-37.80 (19)	C10—C6—C11—N1	-20.3 (4)
C9—Fe1—C6—C7	-81.3 (2)	Fe1—C6—C11—N1	-109.0 (2)
C2—Fe1—C6—C7	164.5 (2)	C7—C6—C11—C12	-21.1 (4)
C4—Fe1—C6—C7	80.3 (2)	C10—C6—C11—C12	158.7 (3)
C1—Fe1—C6—C7	-160.4 (5)	Fe1—C6—C11—C12	70.0 (3)
C5—Fe1—C6—C7	43.7 (4)	N1—C11—C12—O1	-178.5 (2)
C10—Fe1—C6—C7	-118.9 (3)	C6—C11—C12—O1	2.5 (4)
C3—Fe1—C6—C7	123.4 (2)	N1—C11—C12—C13	2.5 (4)
C8—Fe1—C6—C10	81.1 (2)	C6—C11—C12—C13	-176.4 (2)
C9—Fe1—C6—C10	37.6 (2)	O1—C12—C13—C14	-179.0 (3)
C7—Fe1—C6—C10	118.9 (3)	C11—C12—C13—C14	-0.1 (4)
C2—Fe1—C6—C10	-76.6 (3)	C12—C13—C14—C15	-1.4 (4)
C4—Fe1—C6—C10	-160.8 (2)	C11—N1—C15—C14	1.9 (4)
C1—Fe1—C6—C10	-41.5 (6)	C11—N1—C15—C16	-176.7 (2)
C5—Fe1—C6—C10	162.7 (3)	C13—C14—C15—N1	0.5 (4)

C3—Fe1—C6—C10

-117.7 (2)

C13—C14—C15—C16

179.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*

D—H

H···*A*

D···*A*

D—H···*A*

O1—H1···N1ⁱ

0.82

1.96

2.774 (3)

169

C7—H7···O1

0.98

2.39

2.866 (4)

109

Symmetry codes: (i) $x+1/2, -y+3/2, z+1/2$.

Fig. 1

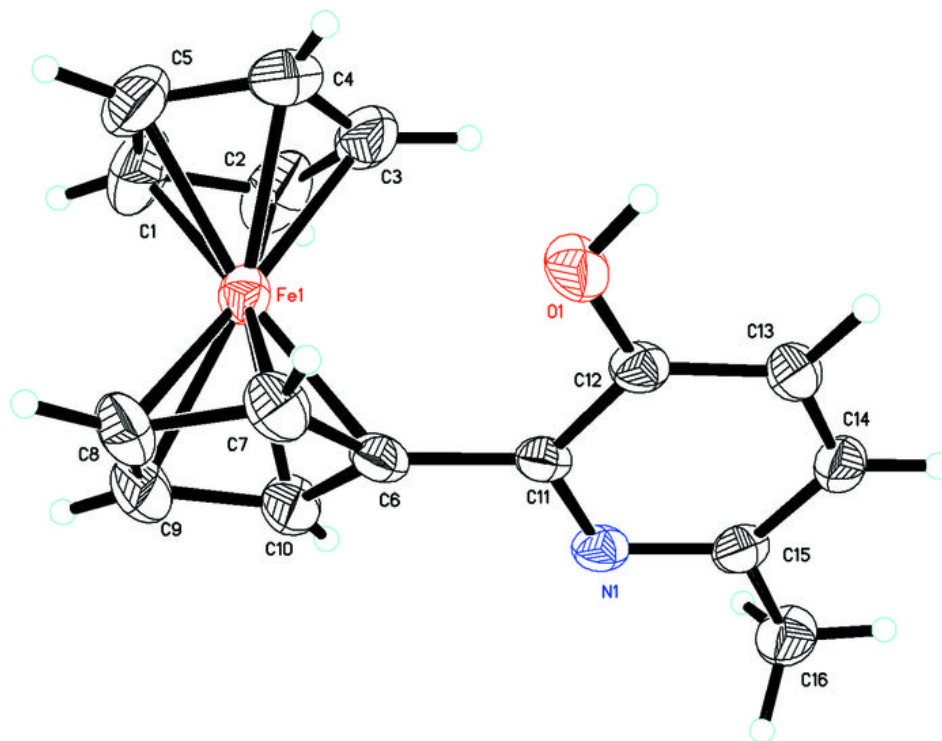


Fig. 2

