Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (*Z*)-3-Ferrocenyl-2-(4-pyridyl)propenenitrile

**Xue-Qun Fu and Wei Wang***

Ordered Matter Science Research Center, Southeast University, Nanjing 210096, People's Republic of China
Correspondence e-mail: seuwangwei@gmail.com

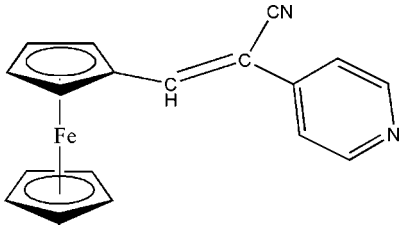
Received 25 June 2008; accepted 22 July 2008

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.049; $wR$ factor = 0.123; data-to-parameter ratio = 17.0.

In the title compound, $[Fe(C_5H_5)(C_{13}H_9N_2)]$, the pyridine ring makes a dihedral angle of 9.91 (17)° with the substituted cyclopentadienyl ring and the double bond adopts a *Z* configuration. In the crystal structure, intermolecular C—H···N hydrogen bonds link the molecules into a one-dimensional chain in the *a*+*c* direction.

## Related literature

For related literature, see: Dupont *et al.* (2005); Shao *et al.* (2005).




## Experimental

### *Crystal data*

$[Fe(C_5H_5)(C_{13}H_9N_2)]$ $M_r$ = 314.16
Monoclinic, $P2_1/n$
$a$ = 11.520 (2) Å
$b$ = 6.0650 (15) Å
$c$ = 20.421 (5) Å
$\beta$ = 91.194 (18)°
$V$ = 1426.5 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.05 mm$^{-1}$
$T$ = 293 (2) K
0.40 × 0.35 × 0.10 mm

### *Data collection*

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.779, $T_{max}$ = 1.000
(expected range = 0.701–0.900)
13960 measured reflections
3229 independent reflections
2543 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.051

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.122
$S$ = 1.05
3229 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.46 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C14—H14$A$···N2$^{i}$ | 0.98 | 2.57 | 3.476 (4) | 153 |

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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 the Starter Fund of Southeast University for financial support to buy the Rigaku SCXmini CCD X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2092).

## References

Dupont, J., Consorti, C. S. & Spencer, J. (2005). *Chem. Rev.* **105**, 2527–2571.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Shao, L., Hu, Y., Tao, W.-F., Jin, Z. & Fang, J.-X. (2005). *Acta Cryst.* E**61**, m1837–m1839.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

# supporting information

*Acta Cryst.* (2008). E**64**, m1072 [doi:10.1107/S1600536808023106]

## (*Z*)-3-Ferrocenyl-2-(4-pyridyl)propenenitrile

**Xue-Qun Fu and Wei Wang**

### S1. Comment

The chemistry of ferrocene has received much attention not only because of its exquisite structure but also its potential applications in many fields such as non-linear optical materials, catalyst and magnetoelectric materials (Dupont *et al.*, 2005). The molecular structure of the title compound is shown in Fig. 1. The C11═C17 bond exhibits a *Z* configuration and the dihedral angle between the pyridine ring and the substituted cyclopentadienyl ring is 9.91 (17)°. The two cyclopentadienyl rings are nearly parallel with the dihedral angle of 3.3 (2)°. The Fe···*Cg*1 and Fe···*Cg*2 distances are 1.6611 (19) Å and 1.6563 (15) Å respectively and the *Cg*1···Fe···*Cg*2 angle is 176.18 (8), where *Cg*1 and *Cg*2 are the centroids of the unsubstituted and substituted Cp rings. Weak intermolecular C—H···N interactions are also found in the crystal structure, which link the compound into one-dimensional chain running in the a+c direction. Similar C—H···N hydrogen bonds in a ferrocene derivative were communicated by Shao *et al.* (2005).

### S2. Experimental

1 ml pyrrolidine was added to the mixture of formylferrocene (2.15 g, 0.01 mol) and 4-pyridineacetonitrile (1.18 g, 0.01 mol) in dichloromethane (100 ml). The mixture was stirred at room temperature for 5 h. After removing the solvent under reduced pressure, the residue was collected and dried in a vacuum desiccator. This crude product was purified by chromatography on silica gel, with petroleum ether and ethyl acetate (10:1 *v*/*v*) as eluent. Brownish red single crystals suitable for X-ray analysis were obtained by slow evaporation of ethanol at room temperature after 24 h.

### S3. Refinement

Positional parameters of all the H atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

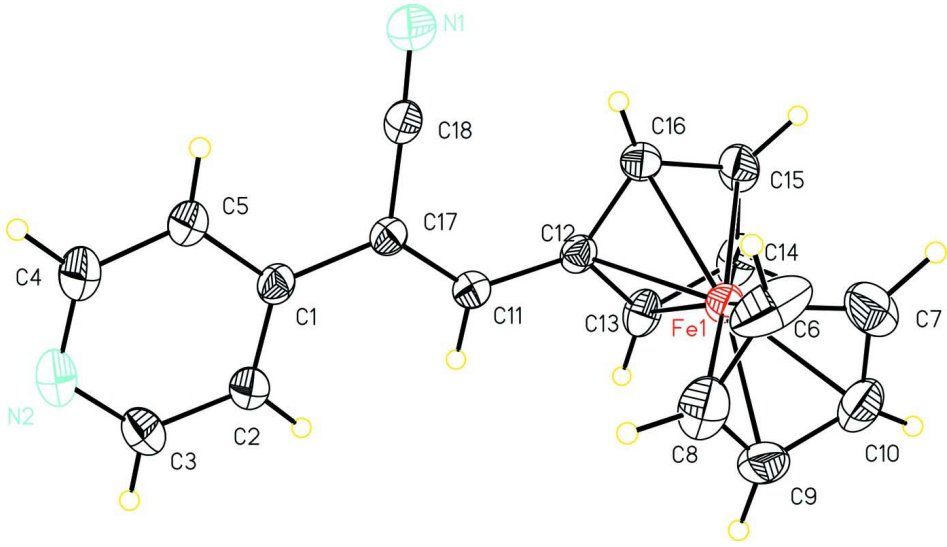



**Figure 1**

Perspective view of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level, and all H atoms have been omitted for clarity.

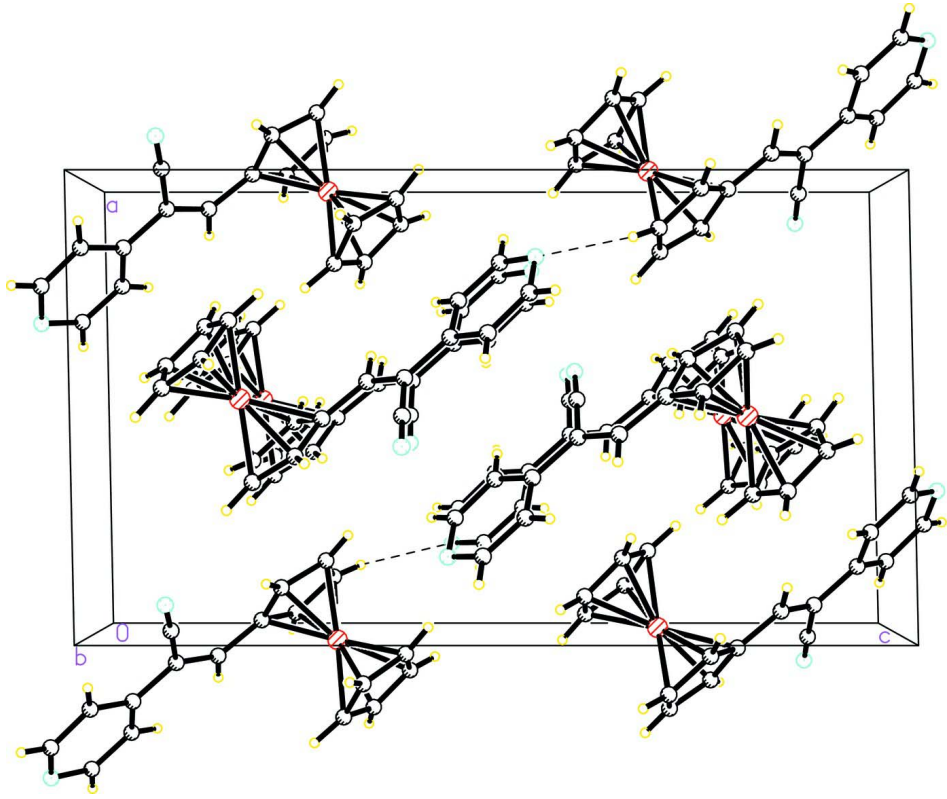



**Figure 2**

Packing of the title compound, viewed along the *b* axis. Dashed lines indicate C—H···N hydrogen-bond interactions.

**(*Z*)-3-Ferrocenyl-2-(4-pyridyl)propenenitrile**

*Crystal data*

$[Fe(C_5H_5)(C_{13}H_9N_2)]$
$M_r = 314.16$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 11.520\ (2)$ Å
$b = 6.0650\ (15)$ Å
$c = 20.421\ (5)$ Å
$\beta = 91.194\ (18)°$
$V = 1426.5\ (6)$ Å$^3$
$Z = 4$
$F(000) = 648$
$D_x = 1.463$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3207 reflections
$\theta = 2.6–27.5°$
$\mu = 1.05$ mm$^{-1}$
$T = 293$ K
Prism, red brown
0.40 × 0.35 × 0.10 mm

*Data collection*

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.779$, $T_{max} = 1.000$
13960 measured reflections
3229 independent reflections
2543 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.5°$
$h = -14\rightarrow14$
$k = -7\rightarrow7$
$l = -26\rightarrow26$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.123$
$S = 1.05$
3229 reflections
190 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
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.4315P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å$^{-3}$
$\Delta\rho_{min} = -0.46$ e Å$^{-3}$

*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 $F^2 > 2\sigma(F^2)$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Fe1 | 0.51801 (3) | 0.90867 (6) | 0.199529 (18) | 0.03900 (15) |
| C12 | 0.4765 (2) | 0.8530 (5) | 0.29581 (12) | 0.0390 (6) |
| C11 | 0.5556 (2) | 0.8741 (5) | 0.35128 (13) | 0.0414 (6) |
| H11A | 0.6106 | 0.7624 | 0.3553 | 0.050* |

| | | | | |
|---|---|---|---|---|
| C17 | 0.5622 (2) | 1.0306 (5) | 0.39804 (12) | 0.0383 (6) |
| C18 | 0.4829 (3) | 1.2149 (5) | 0.39637 (13) | 0.0468 (7) |
| C16 | 0.3975 (2) | 1.0073 (6) | 0.26614 (14) | 0.0473 (7) |
| H16A | 0.3840 | 1.1590 | 0.2807 | 0.057* |
| C15 | 0.3415 (3) | 0.9013 (6) | 0.21203 (16) | 0.0567 (8) |
| H15A | 0.2832 | 0.9684 | 0.1826 | 0.068* |
| C1 | 0.6478 (2) | 1.0312 (5) | 0.45305 (12) | 0.0397 (6) |
| C10 | 0.5885 (3) | 0.8562 (7) | 0.10971 (17) | 0.0654 (10) |
| H10A | 0.5645 | 0.7404 | 0.0788 | 0.079* |
| C5 | 0.6533 (3) | 1.2051 (5) | 0.49758 (14) | 0.0540 (8) |
| H5A | 0.6007 | 1.3211 | 0.4941 | 0.065* |
| C2 | 0.7280 (3) | 0.8635 (5) | 0.46294 (15) | 0.0526 (8) |
| H2A | 0.7274 | 0.7411 | 0.4355 | 0.063* |
| C13 | 0.4691 (3) | 0.6536 (5) | 0.25760 (14) | 0.0496 (7) |
| H13A | 0.5138 | 0.5185 | 0.2658 | 0.060* |
| C7 | 0.5411 (3) | 1.0641 (8) | 0.1125 (2) | 0.0766 (13) |
| H7A | 0.4800 | 1.1236 | 0.0835 | 0.092* |
| N2 | 0.8151 (3) | 1.0472 (6) | 0.55546 (14) | 0.0719 (9) |
| C9 | 0.6729 (3) | 0.8351 (7) | 0.15696 (17) | 0.0628 (9) |
| H9A | 0.7189 | 0.7019 | 0.1654 | 0.075* |
| N1 | 0.4213 (3) | 1.3642 (5) | 0.39676 (15) | 0.0733 (9) |
| C8 | 0.6822 (3) | 1.0285 (8) | 0.19148 (19) | 0.0735 (11) |
| H8A | 0.7371 | 1.0587 | 0.2277 | 0.088* |
| C4 | 0.7369 (3) | 1.2044 (6) | 0.54673 (17) | 0.0683 (10) |
| H4A | 0.7384 | 1.3226 | 0.5758 | 0.082* |
| C14 | 0.3852 (3) | 0.6842 (6) | 0.20690 (15) | 0.0584 (9) |
| H14A | 0.3621 | 0.5750 | 0.1737 | 0.070* |
| C6 | 0.5998 (4) | 1.1787 (6) | 0.1642 (3) | 0.0914 (16) |
| H6A | 0.5877 | 1.3322 | 0.1774 | 0.110* |
| C3 | 0.8088 (3) | 0.8783 (7) | 0.51349 (18) | 0.0696 (10) |
| H3A | 0.8621 | 0.7641 | 0.5187 | 0.084* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Fe1 | 0.0337 (2) | 0.0464 (3) | 0.0369 (2) | −0.00351 (17) | 0.00162 (15) | −0.00326 (17) |
| C12 | 0.0347 (13) | 0.0474 (15) | 0.0352 (13) | −0.0041 (11) | 0.0052 (11) | −0.0042 (11) |
| C11 | 0.0385 (14) | 0.0476 (16) | 0.0381 (14) | 0.0034 (12) | 0.0023 (11) | −0.0023 (12) |
| C17 | 0.0381 (13) | 0.0438 (15) | 0.0331 (13) | 0.0010 (11) | 0.0043 (11) | −0.0007 (11) |
| C18 | 0.0560 (17) | 0.0494 (17) | 0.0350 (14) | 0.0059 (14) | −0.0010 (13) | −0.0052 (12) |
| C16 | 0.0337 (13) | 0.0643 (18) | 0.0439 (16) | 0.0046 (14) | 0.0025 (12) | −0.0034 (14) |
| C15 | 0.0327 (14) | 0.090 (3) | 0.0468 (17) | −0.0094 (16) | −0.0024 (13) | −0.0015 (16) |
| C1 | 0.0403 (14) | 0.0479 (15) | 0.0311 (13) | −0.0009 (12) | 0.0054 (11) | −0.0001 (11) |
| C10 | 0.067 (2) | 0.085 (3) | 0.0450 (18) | −0.007 (2) | 0.0142 (17) | −0.0103 (17) |
| C5 | 0.0583 (18) | 0.0573 (19) | 0.0461 (16) | 0.0090 (15) | −0.0074 (14) | −0.0147 (14) |
| C2 | 0.0554 (18) | 0.0564 (18) | 0.0457 (16) | 0.0118 (14) | −0.0065 (14) | −0.0081 (14) |
| C13 | 0.0584 (18) | 0.0493 (16) | 0.0412 (15) | −0.0135 (14) | 0.0041 (14) | −0.0039 (13) |
| C7 | 0.051 (2) | 0.108 (4) | 0.071 (2) | 0.008 (2) | 0.0099 (18) | 0.045 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2 | 0.076 (2) | 0.089 (2) | 0.0502 (16) | 0.0058 (18) | −0.0193 (15) | −0.0102 (16) |
| C9 | 0.0493 (18) | 0.079 (2) | 0.061 (2) | 0.0138 (17) | 0.0159 (16) | 0.0095 (18) |
| N1 | 0.091 (2) | 0.0681 (19) | 0.0603 (18) | 0.0309 (18) | −0.0086 (17) | −0.0103 (15) |
| C8 | 0.0479 (19) | 0.114 (3) | 0.058 (2) | −0.036 (2) | 0.0079 (17) | −0.008 (2) |
| C4 | 0.073 (2) | 0.074 (2) | 0.057 (2) | 0.006 (2) | −0.0164 (18) | −0.0215 (19) |
| C14 | 0.0529 (18) | 0.077 (2) | 0.0453 (17) | −0.0288 (17) | 0.0042 (14) | −0.0083 (16) |
| C6 | 0.113 (4) | 0.0426 (19) | 0.121 (4) | −0.017 (2) | 0.073 (3) | −0.004 (2) |
| C3 | 0.066 (2) | 0.082 (2) | 0.060 (2) | 0.0230 (19) | −0.0200 (18) | −0.0055 (19) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Fe1—C6 | 2.030 (4) | C1—C5 | 1.393 (4) |
| Fe1—C7 | 2.034 (3) | C10—C9 | 1.361 (5) |
| Fe1—C13 | 2.036 (3) | C10—C7 | 1.376 (5) |
| Fe1—C8 | 2.037 (3) | C10—H10A | 0.9800 |
| Fe1—C10 | 2.046 (3) | C5—C4 | 1.376 (4) |
| Fe1—C9 | 2.050 (3) | C5—H5A | 0.9300 |
| Fe1—C16 | 2.053 (3) | C2—C3 | 1.378 (5) |
| Fe1—C15 | 2.055 (3) | C2—H2A | 0.9300 |
| Fe1—C14 | 2.056 (3) | C13—C14 | 1.414 (4) |
| Fe1—C12 | 2.061 (3) | C13—H13A | 0.9800 |
| C12—C16 | 1.431 (4) | C7—C6 | 1.423 (6) |
| C12—C13 | 1.441 (4) | C7—H7A | 0.9800 |
| C12—C11 | 1.445 (4) | N2—C4 | 1.321 (5) |
| C11—C17 | 1.347 (4) | N2—C3 | 1.336 (5) |
| C11—H11A | 0.9300 | C9—C8 | 1.371 (6) |
| C17—C18 | 1.443 (4) | C9—H9A | 0.9800 |
| C17—C1 | 1.480 (4) | C8—C6 | 1.421 (6) |
| C18—N1 | 1.150 (4) | C8—H8A | 0.9800 |
| C16—C15 | 1.422 (4) | C4—H4A | 0.9300 |
| C16—H16A | 0.9800 | C14—H14A | 0.9800 |
| C15—C14 | 1.414 (5) | C6—H6A | 0.9800 |
| C15—H15A | 0.9800 | C3—H3A | 0.9300 |
| C1—C2 | 1.386 (4) | | |

| | | | |
|---|---|---|---|
| C6—Fe1—C7 | 40.99 (18) | C14—C15—C16 | 108.8 (3) |
| C6—Fe1—C13 | 163.0 (2) | C14—C15—Fe1 | 69.91 (17) |
| C7—Fe1—C13 | 154.67 (17) | C16—C15—Fe1 | 69.67 (16) |
| C6—Fe1—C8 | 40.91 (19) | C14—C15—H15A | 125.6 |
| C7—Fe1—C8 | 68.01 (16) | C16—C15—H15A | 125.6 |
| C13—Fe1—C8 | 125.95 (17) | Fe1—C15—H15A | 125.6 |
| C6—Fe1—C10 | 67.09 (16) | C2—C1—C5 | 116.1 (3) |
| C7—Fe1—C10 | 39.40 (16) | C2—C1—C17 | 122.7 (3) |
| C13—Fe1—C10 | 121.59 (14) | C5—C1—C17 | 121.2 (3) |
| C8—Fe1—C10 | 66.19 (15) | C9—C10—C7 | 109.6 (4) |
| C6—Fe1—C9 | 67.04 (16) | C9—C10—Fe1 | 70.72 (19) |
| C7—Fe1—C9 | 66.39 (15) | C7—C10—Fe1 | 69.8 (2) |
| C13—Fe1—C9 | 109.61 (14) | C9—C10—H10A | 125.2 |

| | | | |
|---|---|---|---|
| C8—Fe1—C9 | 39.21 (16) | C7—C10—H10A | 125.2 |
| C10—Fe1—C9 | 38.82 (14) | Fe1—C10—H10A | 125.2 |
| C6—Fe1—C16 | 109.02 (14) | C4—C5—C1 | 119.7 (3) |
| C7—Fe1—C16 | 123.12 (15) | C4—C5—H5A | 120.2 |
| C13—Fe1—C16 | 68.68 (14) | C1—C5—H5A | 120.2 |
| C8—Fe1—C16 | 126.27 (15) | C3—C2—C1 | 119.9 (3) |
| C10—Fe1—C16 | 157.78 (14) | C3—C2—H2A | 120.0 |
| C9—Fe1—C16 | 161.98 (14) | C1—C2—H2A | 120.0 |
| C6—Fe1—C15 | 122.00 (18) | C14—C13—C12 | 108.5 (3) |
| C7—Fe1—C15 | 105.45 (14) | C14—C13—Fe1 | 70.54 (18) |
| C13—Fe1—C15 | 67.94 (14) | C12—C13—Fe1 | 70.35 (16) |
| C8—Fe1—C15 | 160.24 (18) | C14—C13—H13A | 125.7 |
| C10—Fe1—C15 | 121.34 (14) | C12—C13—H13A | 125.7 |
| C9—Fe1—C15 | 156.93 (15) | Fe1—C13—H13A | 125.7 |
| C16—Fe1—C15 | 40.50 (12) | C10—C7—C6 | 107.2 (4) |
| C6—Fe1—C14 | 155.8 (2) | C10—C7—Fe1 | 70.8 (2) |
| C7—Fe1—C14 | 118.82 (16) | C6—C7—Fe1 | 69.3 (2) |
| C13—Fe1—C14 | 40.42 (13) | C10—C7—H7A | 126.4 |
| C8—Fe1—C14 | 159.43 (18) | C6—C7—H7A | 126.4 |
| C10—Fe1—C14 | 105.82 (14) | Fe1—C7—H7A | 126.4 |
| C9—Fe1—C14 | 122.86 (16) | C4—N2—C3 | 116.0 (3) |
| C16—Fe1—C14 | 68.28 (14) | C10—C9—C8 | 109.4 (4) |
| C15—Fe1—C14 | 40.23 (14) | C10—C9—Fe1 | 70.5 (2) |
| C6—Fe1—C12 | 126.17 (16) | C8—C9—Fe1 | 69.9 (2) |
| C7—Fe1—C12 | 161.19 (16) | C10—C9—H9A | 125.3 |
| C13—Fe1—C12 | 41.18 (11) | C8—C9—H9A | 125.3 |
| C8—Fe1—C12 | 111.72 (13) | Fe1—C9—H9A | 125.3 |
| C10—Fe1—C12 | 159.07 (14) | C9—C8—C6 | 107.6 (4) |
| C9—Fe1—C12 | 126.18 (13) | C9—C8—Fe1 | 70.9 (2) |
| C16—Fe1—C12 | 40.71 (11) | C6—C8—Fe1 | 69.3 (2) |
| C15—Fe1—C12 | 68.16 (12) | C9—C8—H8A | 126.2 |
| C14—Fe1—C12 | 68.51 (11) | C6—C8—H8A | 126.2 |
| C16—C12—C13 | 106.9 (3) | Fe1—C8—H8A | 126.2 |
| C16—C12—C11 | 131.2 (3) | N2—C4—C5 | 124.4 (3) |
| C13—C12—C11 | 121.9 (3) | N2—C4—H4A | 117.8 |
| C16—C12—Fe1 | 69.33 (16) | C5—C4—H4A | 117.8 |
| C13—C12—Fe1 | 68.48 (15) | C13—C14—C15 | 107.9 (3) |
| C11—C12—Fe1 | 125.30 (18) | C13—C14—Fe1 | 69.05 (17) |
| C17—C11—C12 | 130.0 (3) | C15—C14—Fe1 | 69.85 (18) |
| C17—C11—H11A | 115.0 | C13—C14—H14A | 126.1 |
| C12—C11—H11A | 115.0 | C15—C14—H14A | 126.1 |
| C11—C17—C18 | 120.2 (3) | Fe1—C14—H14A | 126.1 |
| C11—C17—C1 | 124.5 (3) | C8—C6—C7 | 106.3 (3) |
| C18—C17—C1 | 115.3 (2) | C8—C6—Fe1 | 69.8 (2) |
| N1—C18—C17 | 177.9 (3) | C7—C6—Fe1 | 69.7 (2) |
| C15—C16—C12 | 107.9 (3) | C8—C6—H6A | 126.8 |
| C15—C16—Fe1 | 69.83 (17) | C7—C6—H6A | 126.8 |
| C12—C16—Fe1 | 69.96 (15) | Fe1—C6—H6A | 126.8 |

| | | | |
|---|---|---|---|
| C15—C16—H16A | 126.1 | N2—C3—C2 | 123.9 (3) |
| C12—C16—H16A | 126.1 | N2—C3—H3A | 118.1 |
| Fe1—C16—H16A | 126.1 | C2—C3—H3A | 118.1 |
| | | | |
| C6—Fe1—C12—C16 | 76.7 (3) | C10—Fe1—C13—C12 | 164.24 (18) |
| C7—Fe1—C12—C16 | 35.5 (5) | C9—Fe1—C13—C12 | 123.00 (19) |
| C13—Fe1—C12—C16 | −118.8 (3) | C16—Fe1—C13—C12 | −37.84 (16) |
| C8—Fe1—C12—C16 | 120.9 (2) | C15—Fe1—C13—C12 | −81.58 (19) |
| C10—Fe1—C12—C16 | −159.2 (3) | C14—Fe1—C13—C12 | −119.0 (3) |
| C9—Fe1—C12—C16 | 163.0 (2) | C9—C10—C7—C6 | 0.3 (4) |
| C15—Fe1—C12—C16 | −37.80 (19) | Fe1—C10—C7—C6 | 60.1 (2) |
| C14—Fe1—C12—C16 | −81.2 (2) | C9—C10—C7—Fe1 | −59.7 (2) |
| C6—Fe1—C12—C13 | −164.5 (2) | C6—Fe1—C7—C10 | 117.8 (3) |
| C7—Fe1—C12—C13 | 154.3 (4) | C13—Fe1—C7—C10 | −50.0 (4) |
| C8—Fe1—C12—C13 | −120.3 (2) | C8—Fe1—C7—C10 | 78.8 (3) |
| C10—Fe1—C12—C13 | −40.4 (4) | C9—Fe1—C7—C10 | 36.1 (2) |
| C9—Fe1—C12—C13 | −78.2 (2) | C16—Fe1—C7—C10 | −161.3 (2) |
| C16—Fe1—C12—C13 | 118.8 (3) | C15—Fe1—C7—C10 | −120.9 (2) |
| C15—Fe1—C12—C13 | 81.0 (2) | C14—Fe1—C7—C10 | −79.7 (3) |
| C14—Fe1—C12—C13 | 37.6 (2) | C12—Fe1—C7—C10 | 171.8 (3) |
| C6—Fe1—C12—C11 | −49.9 (3) | C13—Fe1—C7—C6 | −167.7 (3) |
| C7—Fe1—C12—C11 | −91.0 (5) | C8—Fe1—C7—C6 | −38.9 (2) |
| C13—Fe1—C12—C11 | 114.6 (3) | C10—Fe1—C7—C6 | −117.8 (3) |
| C8—Fe1—C12—C11 | −5.7 (3) | C9—Fe1—C7—C6 | −81.6 (3) |
| C10—Fe1—C12—C11 | 74.3 (5) | C16—Fe1—C7—C6 | 80.9 (3) |
| C9—Fe1—C12—C11 | 36.4 (3) | C15—Fe1—C7—C6 | 121.3 (3) |
| C16—Fe1—C12—C11 | −126.6 (3) | C14—Fe1—C7—C6 | 162.6 (2) |
| C15—Fe1—C12—C11 | −164.4 (3) | C12—Fe1—C7—C6 | 54.0 (5) |
| C14—Fe1—C12—C11 | 152.2 (3) | C7—C10—C9—C8 | 0.0 (4) |
| C16—C12—C11—C17 | 14.0 (5) | Fe1—C10—C9—C8 | −59.2 (2) |
| C13—C12—C11—C17 | −168.5 (3) | C7—C10—C9—Fe1 | 59.2 (2) |
| Fe1—C12—C11—C17 | 106.6 (3) | C6—Fe1—C9—C10 | −81.5 (3) |
| C12—C11—C17—C18 | −1.2 (5) | C7—Fe1—C9—C10 | −36.7 (3) |
| C12—C11—C17—C1 | 179.4 (3) | C13—Fe1—C9—C10 | 116.4 (2) |
| C13—C12—C16—C15 | 1.4 (3) | C8—Fe1—C9—C10 | −120.3 (4) |
| C11—C12—C16—C15 | 179.2 (3) | C16—Fe1—C9—C10 | −162.4 (4) |
| Fe1—C12—C16—C15 | 59.8 (2) | C15—Fe1—C9—C10 | 36.8 (5) |
| C13—C12—C16—Fe1 | −58.40 (19) | C14—Fe1—C9—C10 | 73.4 (3) |
| C11—C12—C16—Fe1 | 119.4 (3) | C12—Fe1—C9—C10 | 159.5 (2) |
| C6—Fe1—C16—C15 | 117.3 (3) | C6—Fe1—C9—C8 | 38.8 (3) |
| C7—Fe1—C16—C15 | 74.1 (3) | C7—Fe1—C9—C8 | 83.6 (3) |
| C13—Fe1—C16—C15 | −80.6 (2) | C13—Fe1—C9—C8 | −123.3 (2) |
| C8—Fe1—C16—C15 | 159.7 (2) | C10—Fe1—C9—C8 | 120.3 (4) |
| C10—Fe1—C16—C15 | 41.5 (5) | C16—Fe1—C9—C8 | −42.1 (6) |
| C9—Fe1—C16—C15 | −168.5 (4) | C15—Fe1—C9—C8 | 157.1 (4) |
| C14—Fe1—C16—C15 | −37.0 (2) | C14—Fe1—C9—C8 | −166.2 (2) |
| C12—Fe1—C16—C15 | −118.8 (3) | C12—Fe1—C9—C8 | −80.1 (3) |
| C6—Fe1—C16—C12 | −123.8 (2) | C10—C9—C8—C6 | −0.3 (4) |

| | | | |
|---|---|---|---|
| C7—Fe1—C16—C12 | −167.1 (2) | Fe1—C9—C8—C6 | −59.9 (2) |
| C13—Fe1—C16—C12 | 38.27 (17) | C10—C9—C8—Fe1 | 59.6 (3) |
| C8—Fe1—C16—C12 | −81.4 (3) | C6—Fe1—C8—C9 | −118.2 (3) |
| C10—Fe1—C16—C12 | 160.4 (4) | C7—Fe1—C8—C9 | −79.1 (3) |
| C9—Fe1—C16—C12 | −49.7 (5) | C13—Fe1—C8—C9 | 76.5 (3) |
| C15—Fe1—C16—C12 | 118.8 (3) | C10—Fe1—C8—C9 | −36.3 (2) |
| C14—Fe1—C16—C12 | 81.86 (19) | C16—Fe1—C8—C9 | 165.1 (2) |
| C12—C16—C15—C14 | −0.7 (3) | C15—Fe1—C8—C9 | −153.2 (4) |
| Fe1—C16—C15—C14 | 59.1 (2) | C14—Fe1—C8—C9 | 34.6 (5) |
| C12—C16—C15—Fe1 | −59.86 (19) | C12—Fe1—C8—C9 | 121.1 (2) |
| C6—Fe1—C15—C14 | 157.9 (2) | C7—Fe1—C8—C6 | 39.0 (3) |
| C7—Fe1—C15—C14 | 116.6 (2) | C13—Fe1—C8—C6 | −165.3 (2) |
| C13—Fe1—C15—C14 | −37.55 (18) | C10—Fe1—C8—C6 | 81.9 (3) |
| C8—Fe1—C15—C14 | −175.7 (4) | C9—Fe1—C8—C6 | 118.2 (3) |
| C10—Fe1—C15—C14 | 77.0 (2) | C16—Fe1—C8—C6 | −76.7 (3) |
| C9—Fe1—C15—C14 | 50.9 (4) | C15—Fe1—C8—C6 | −35.1 (5) |
| C16—Fe1—C15—C14 | −120.1 (3) | C14—Fe1—C8—C6 | 152.8 (4) |
| C12—Fe1—C15—C14 | −82.1 (2) | C12—Fe1—C8—C6 | −120.7 (3) |
| C6—Fe1—C15—C16 | −82.0 (3) | C3—N2—C4—C5 | −1.1 (6) |
| C7—Fe1—C15—C16 | −123.3 (2) | C1—C5—C4—N2 | 0.0 (6) |
| C13—Fe1—C15—C16 | 82.6 (2) | C12—C13—C14—C15 | 1.1 (3) |
| C8—Fe1—C15—C16 | −55.6 (5) | Fe1—C13—C14—C15 | −59.3 (2) |
| C10—Fe1—C15—C16 | −162.9 (2) | C12—C13—C14—Fe1 | 60.35 (19) |
| C9—Fe1—C15—C16 | 171.0 (3) | C16—C15—C14—C13 | −0.2 (3) |
| C14—Fe1—C15—C16 | 120.1 (3) | Fe1—C15—C14—C13 | 58.8 (2) |
| C12—Fe1—C15—C16 | 37.99 (19) | C16—C15—C14—Fe1 | −59.0 (2) |
| C11—C17—C1—C2 | −2.4 (4) | C6—Fe1—C14—C13 | −170.4 (3) |
| C18—C17—C1—C2 | 178.2 (3) | C7—Fe1—C14—C13 | 160.9 (2) |
| C11—C17—C1—C5 | 176.5 (3) | C8—Fe1—C14—C13 | 56.5 (4) |
| C18—C17—C1—C5 | −3.0 (4) | C10—Fe1—C14—C13 | 120.5 (2) |
| C6—Fe1—C10—C9 | 81.4 (3) | C9—Fe1—C14—C13 | 81.8 (2) |
| C7—Fe1—C10—C9 | 120.4 (4) | C16—Fe1—C14—C13 | −82.2 (2) |
| C13—Fe1—C10—C9 | −82.2 (3) | C15—Fe1—C14—C13 | −119.4 (3) |
| C8—Fe1—C10—C9 | 36.6 (3) | C12—Fe1—C14—C13 | −38.25 (18) |
| C16—Fe1—C10—C9 | 165.7 (3) | C6—Fe1—C14—C15 | −51.0 (4) |
| C15—Fe1—C10—C9 | −164.0 (2) | C7—Fe1—C14—C15 | −79.7 (2) |
| C14—Fe1—C10—C9 | −123.2 (2) | C13—Fe1—C14—C15 | 119.4 (3) |
| C12—Fe1—C10—C9 | −52.2 (5) | C8—Fe1—C14—C15 | 175.9 (4) |
| C6—Fe1—C10—C7 | −39.1 (3) | C10—Fe1—C14—C15 | −120.1 (2) |
| C13—Fe1—C10—C7 | 157.4 (2) | C9—Fe1—C14—C15 | −158.78 (19) |
| C8—Fe1—C10—C7 | −83.8 (3) | C16—Fe1—C14—C15 | 37.22 (19) |
| C9—Fe1—C10—C7 | −120.4 (4) | C12—Fe1—C14—C15 | 81.2 (2) |
| C16—Fe1—C10—C7 | 45.3 (5) | C9—C8—C6—C7 | 0.5 (4) |
| C15—Fe1—C10—C7 | 75.5 (3) | Fe1—C8—C6—C7 | −60.4 (2) |
| C14—Fe1—C10—C7 | 116.4 (3) | C9—C8—C6—Fe1 | 60.9 (2) |
| C12—Fe1—C10—C7 | −172.6 (3) | C10—C7—C6—C8 | −0.5 (4) |
| C2—C1—C5—C4 | 1.4 (5) | Fe1—C7—C6—C8 | 60.5 (3) |
| C17—C1—C5—C4 | −177.6 (3) | C10—C7—C6—Fe1 | −61.0 (2) |

| | | | |
|---|---|---|---|
| C5—C1—C2—C3 | −1.7 (5) | C7—Fe1—C6—C8 | −117.1 (3) |
| C17—C1—C2—C3 | 177.2 (3) | C13—Fe1—C6—C8 | 44.7 (6) |
| C16—C12—C13—C14 | −1.5 (3) | C10—Fe1—C6—C8 | −79.6 (3) |
| C11—C12—C13—C14 | −179.6 (2) | C9—Fe1—C6—C8 | −37.2 (2) |
| Fe1—C12—C13—C14 | −60.5 (2) | C16—Fe1—C6—C8 | 123.9 (2) |
| C16—C12—C13—Fe1 | 58.94 (19) | C15—Fe1—C6—C8 | 166.8 (2) |
| C11—C12—C13—Fe1 | −119.1 (2) | C14—Fe1—C6—C8 | −156.9 (3) |
| C6—Fe1—C13—C14 | 166.5 (5) | C12—Fe1—C6—C8 | 81.7 (3) |
| C7—Fe1—C13—C14 | −42.0 (4) | C13—Fe1—C6—C7 | 161.9 (4) |
| C8—Fe1—C13—C14 | −158.8 (2) | C8—Fe1—C6—C7 | 117.1 (3) |
| C10—Fe1—C13—C14 | −76.8 (2) | C10—Fe1—C6—C7 | 37.6 (2) |
| C9—Fe1—C13—C14 | −118.0 (2) | C9—Fe1—C6—C7 | 79.9 (2) |
| C16—Fe1—C13—C14 | 81.1 (2) | C16—Fe1—C6—C7 | −119.0 (2) |
| C15—Fe1—C13—C14 | 37.38 (19) | C15—Fe1—C6—C7 | −76.1 (3) |
| C12—Fe1—C13—C14 | 119.0 (3) | C14—Fe1—C6—C7 | −39.8 (5) |
| C6—Fe1—C13—C12 | 47.5 (6) | C12—Fe1—C6—C7 | −161.1 (2) |
| C7—Fe1—C13—C12 | −161.0 (3) | C4—N2—C3—C2 | 0.8 (6) |
| C8—Fe1—C13—C12 | 82.3 (2) | C1—C2—C3—N2 | 0.7 (6) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14*A*···N2$^{i}$ | 0.98 | 2.57 | 3.476 (4) | 153 |

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