

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

cis-Bis(2,2'-bipyridine- κ^2N,N')-dichloridoiron(III) perchlorate

Zhi-Fang Zhang

School of Chemistry and Chemical Engineering, Yulin University, Yulin 719000, People's Republic of China

Correspondence e-mail: zhi.fang889@126.com

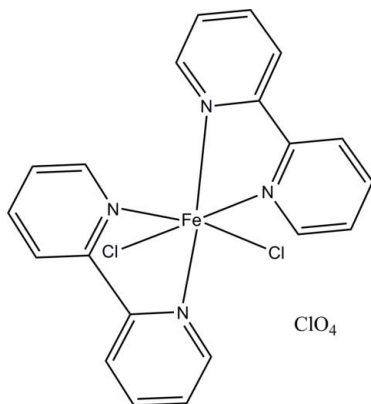
Received 11 April 2011; accepted 27 April 2011

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.011$ Å; R factor = 0.063; wR factor = 0.125; data-to-parameter ratio = 12.2.

In the crystal structure of the title compound, $[\text{FeCl}_2(\text{C}_{10}\text{H}_8\text{N}_2)_2]\text{ClO}_4$, the coordination around the Fe^{III} atom is approximately octahedral. The equatorial positions are occupied by two N atoms from two 2,2'-bipyridyl ligands [$\text{Fe}-\text{N} = 2.121$ (5) and 2.147 (5) Å] and two Cl atoms [$\text{Fe}-\text{Cl} = 2.220$ (2) and 2.2074 (18) Å]. Weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Cl}$ hydrogen bonds and $\text{C}-\text{H}\cdots\pi$ interactions consolidate the crystal packing.

Related literature

For the use of bipyridine and analogous ligands in the formation of transition metal complexes, see: Constable (1989). For applications of related compounds, see: Constable & Steel (1989); Steel *et al.* (1990). For related structures, see: Amani *et al.* (2007); Figgis *et al.* (1983).



Experimental

Crystal data

$[\text{FeCl}_2(\text{C}_{10}\text{H}_8\text{N}_2)_2]\text{ClO}_4$ $a = 10.891$ (2) Å
 $M_r = 538.57$ $b = 11.522$ (2) Å
 Orthorhombic, $P2_12_12_1$ $c = 16.990$ (3) Å

$V = 2132.1$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 1.12$ mm⁻¹
 $T = 295$ K
 $0.34 \times 0.29 \times 0.24$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer 5914 measured reflections
 3534 independent reflections
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003) 2810 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$
 $T_{\text{min}} = 0.702$, $T_{\text{max}} = 0.775$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.063$ $\Delta\rho_{\text{max}} = 0.75$ e Å⁻³
 $wR(F^2) = 0.125$ $\Delta\rho_{\text{min}} = -0.42$ e Å⁻³
 $S = 1.08$ Absolute structure: Flack (1983),
 3534 reflections 1419 Friedel pairs
 289 parameters Flack parameter: 0.05 (3)
 H-atom parameters constrained

Table 1

Hydrogen-bond geometry (Å, °).

Cg4 is the centroid of the N2,C6-C10 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3-H3 \cdots O2	0.93	2.52	3.140 (11)	124
C7-H7 \cdots O3 ⁱ	0.93	2.55	3.239 (9)	131
C8-H8 \cdots O2 ⁱⁱ	0.93	2.30	3.152 (9)	152
C13-H13 \cdots O2 ⁱⁱⁱ	0.93	2.54	3.423 (10)	158
C18-H18 \cdots O4 ^{iv}	0.93	2.51	3.387 (10)	158
C10-H10 \cdots Cl3	0.93	2.71	3.308 (7)	122
C20-H20 \cdots Cl2	0.93	2.79	3.382 (7)	123
C11-H11 \cdots Cg4	0.93	2.90	3.705 (8)	146

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{3}{2}, -z$; (ii) $-x + \frac{3}{2}, -y + 1, z - \frac{1}{2}$; (iii) $x + 1, y, z$; (iv) $-x + \frac{3}{2}, -y + 1, z + \frac{1}{2}$.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2003); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

The author gratefully acknowledges financial support from the Natural Science Foundation of the Education Department of Shaanxi Provincial Government (09 J K844) and is grateful for support provided by the key industry problem plan of Yulin (gygg200807) and the special research projects of Yulin University (08YK17).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2098).

References

- Amani, V., Safari, N. & Khavasi, H. R. (2007). *Polyhedron*, **26**, 4257–4262.
 Bruker (2001). SMART. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (2003). SAINT-Plus. Bruker AXS Inc., Madison, Wisconsin, USA.
 Constable, E. C. (1989). *Adv. Inorg. Chem.* **34**, 1–63.
 Constable, E. C. & Steel, P. J. (1989). *Coord. Chem. Rev.* **93**, 205–223.
 Figgis, B. N., Reynolds, P. A. & Lehner, N. (1983). *Acta Cryst.* **B39**, 711–717.
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Sheldrick, G. M. (2003). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Steel, P. J. (1990). *Coord. Chem. Rev.* **106**, 227–265.

supplementary materials

Acta Cryst. (2011). E67, m677 [doi:10.1107/S1600536811016035]

cis-Bis(2,2'-bipyridine- κ^2N,N')dichloridoiron(III) perchlorate

Z.-F. Zhang

Comment

Bipyridine and analogous ligands such as phenanthroline are commonly used in the formation of different complexes with a general variety of transition metals (Constable, 1989). Studies of these transition metal complexes are important in understanding electron transfer processes, mixed valence complexes, magnetic coupling and magnetic transitions (Constable *et al.*, 1989; Steel *et al.*, 1990). Although bipyridine coordination to iron has been widely investigated, most complexes are iron(II) complexes, little attention has been paid to bipyridine iron(III) complexes. In order to expand this field, the title compound has been synthesized, and its crystal structure is reported herein.

The molecular structure of the title compound (I) is shown in Fig. 1. The crystal is composed of *cis*-[Fe^{III}(bipy)₂Cl₂]⁺ cations and [ClO₄]⁻ anions. The Fe^{III} atom is coordinated by two Cl anions and four N atoms from two 2,2'-bipyridyl ligands within a distorted octahedral geometry. The six-coordinate molecule is the *cis-cis* isomer considering the positions of the chlorine and pyridyl nitrogen atoms. The four Fe—N bond lengths [2.087 (4)–2.147 (5) Å] were similar and consistent with those reported earlier (Amani *et al.*, 2007; Figgis *et al.*, 1983). The distortion from a perfect octahedral geometry was primarily a consequence of the small bite-angle of the chelating ligands, which led to acute N1—Fe—N2 and N3—Fe—N4 angles of 75.96 (19)° and 75.4 (2)°, respectively.

Intermolecular C—H \cdots O, C—H \cdots Cl hydrogen bonds and C—H \cdots π interactions stabilize the crystal structure (Table 1).

Experimental

All reagents were obtained from commercial sources and used without further purification. 2,2'-Bipyridine (0.312 g, 2.0 mmol) and NaClO₄ (0.122 g, 1.0 mmol) were added to a solution of FeCl₃·6H₂O (0.270 g, 1.0 mmol) in methanol (30 ml), and the solution was stirred at 60–65 °C for 3 h. A red-brown precipitate was obtained. After filtration, the red-brown filtrate was allowed to stand at room temperature for two weeks to give red-brown block-shaped crystals suitable for X-ray analysis. Elemental analysis for C₂₀H₁₆Cl₃FeN₄O₄: C 44.60, H 2.99, N 10.40 %; found: C 44.52, H 3.03, N 10.39 %.

Refinement

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

Figures

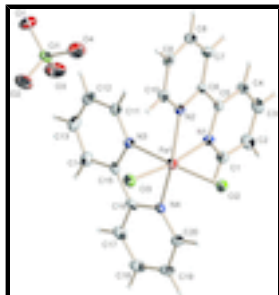


Fig. 1. The molecular structure of the title compound showing thermal ellipsoids at the 30% probability level.

cis-Bis(2,2'-bipyridine- κ^2N,N')dichloridoiron(III) perchlorate

Crystal data

[FeCl₂(C₁₀H₈N₂)₂]ClO₄

$M_r = 538.57$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 10.891$ (2) Å

$b = 11.522$ (2) Å

$c = 16.990$ (3) Å

$V = 2132.1$ (7) Å³

$Z = 4$

$F(000) = 1092$

$D_x = 1.678$ Mg m⁻³

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

Cell parameters from 1783 reflections

$\theta = 2.4$ – 25.9°

$\mu = 1.12$ mm⁻¹

$T = 295$ K

Block, red-brown

$0.34 \times 0.29 \times 0.24$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)

$T_{\min} = 0.702$, $T_{\max} = 0.775$

5914 measured reflections

3534 independent reflections

2810 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 3.0^\circ$

$h = -7 \rightarrow 12$

$k = -12 \rightarrow 13$

$l = -20 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.063$

$wR(F^2) = 0.125$

$S = 1.08$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.4377P]$

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

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

3534 reflections	$\Delta\rho_{\max} = 0.75 \text{ e } \text{\AA}^{-3}$
289 parameters	$\Delta\rho_{\min} = -0.42 \text{ e } \text{\AA}^{-3}$
0 restraints	Absolute structure: Flack (1983), 1419 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.05 (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 $F^2 > \sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
Fe1	0.97563 (9)	0.23098 (7)	0.13357 (5)	0.0557 (3)
Cl1	0.4647 (2)	0.80918 (14)	0.13791 (10)	0.0674 (5)
Cl2	0.79726 (18)	0.13772 (13)	0.13412 (11)	0.0693 (5)
Cl3	1.10061 (18)	0.08017 (14)	0.13284 (11)	0.0722 (5)
O1	0.5403 (7)	0.8608 (5)	0.0835 (3)	0.111 (2)
O2	0.5221 (7)	0.7174 (5)	0.1726 (3)	0.127 (2)
O3	0.4321 (8)	0.8861 (5)	0.1958 (3)	0.139 (3)
O4	0.3639 (7)	0.7708 (8)	0.0978 (4)	0.164 (3)
N1	0.8727 (5)	0.3863 (4)	0.1221 (3)	0.0511 (13)
N2	0.9729 (5)	0.2621 (4)	0.0126 (3)	0.0499 (12)
N3	1.1301 (5)	0.3461 (4)	0.1420 (3)	0.0551 (13)
N4	0.9974 (5)	0.2596 (4)	0.2546 (3)	0.0529 (13)
C1	0.8236 (7)	0.4446 (6)	0.1798 (4)	0.067 (2)
H1	0.8394	0.4209	0.2311	0.080*
C2	0.7503 (8)	0.5385 (6)	0.1681 (5)	0.079 (3)
H2	0.7126	0.5762	0.2101	0.095*
C3	0.7341 (8)	0.5753 (6)	0.0926 (5)	0.076 (2)
H3	0.6866	0.6406	0.0823	0.092*
C4	0.7870 (8)	0.5169 (6)	0.0333 (4)	0.065 (2)
H4	0.7762	0.5419	-0.0183	0.078*
C5	0.8558 (6)	0.4220 (5)	0.0484 (4)	0.0481 (15)
C6	0.9143 (6)	0.3543 (5)	-0.0115 (3)	0.0475 (15)
C7	0.9110 (8)	0.3798 (6)	-0.0911 (4)	0.067 (2)
H7	0.8674	0.4442	-0.1086	0.081*
C8	0.9698 (7)	0.3129 (7)	-0.1431 (4)	0.073 (2)
H8	0.9702	0.3321	-0.1963	0.087*
C9	1.0269 (7)	0.2198 (6)	-0.1181 (4)	0.0691 (19)

supplementary materials

H9	1.0661	0.1710	-0.1538	0.083*
C10	1.0287 (7)	0.1949 (5)	-0.0396 (4)	0.0604 (17)
H10	1.0701	0.1291	-0.0223	0.072*
C11	1.1910 (7)	0.3941 (6)	0.0843 (4)	0.0658 (19)
H11	1.1659	0.3775	0.0333	0.079*
C12	1.2875 (9)	0.4658 (6)	0.0934 (5)	0.079 (2)
H12	1.3255	0.5006	0.0504	0.094*
C13	1.3264 (8)	0.4850 (6)	0.1671 (5)	0.079 (2)
H13	1.3935	0.5331	0.1762	0.095*
C14	1.2681 (8)	0.4344 (6)	0.2280 (4)	0.070 (2)
H14	1.2965	0.4458	0.2790	0.084*
C15	1.1680 (7)	0.3669 (5)	0.2151 (4)	0.0533 (16)
C16	1.0945 (7)	0.3178 (5)	0.2775 (4)	0.0564 (18)
C17	1.1226 (8)	0.3310 (5)	0.3553 (4)	0.072 (2)
H17	1.1922	0.3722	0.3703	0.087*
C18	1.0481 (10)	0.2833 (7)	0.4102 (4)	0.085 (3)
H18	1.0670	0.2904	0.4633	0.102*
C19	0.9466 (9)	0.2257 (7)	0.3879 (4)	0.086 (3)
H19	0.8932	0.1947	0.4251	0.104*
C20	0.9236 (8)	0.2136 (6)	0.3085 (4)	0.078 (2)
H20	0.8548	0.1722	0.2923	0.094*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0563 (6)	0.0609 (5)	0.0499 (5)	0.0006 (5)	-0.0004 (5)	0.0042 (4)
Cl1	0.0817 (14)	0.0688 (9)	0.0518 (9)	0.0106 (10)	-0.0023 (11)	0.0058 (9)
Cl2	0.0587 (11)	0.0678 (9)	0.0814 (11)	-0.0092 (8)	-0.0010 (11)	0.0118 (10)
Cl3	0.0703 (13)	0.0697 (9)	0.0765 (11)	0.0135 (9)	-0.0031 (11)	0.0088 (10)
O1	0.126 (6)	0.117 (4)	0.089 (3)	-0.022 (4)	0.033 (4)	0.012 (3)
O2	0.152 (7)	0.112 (4)	0.117 (4)	0.065 (5)	0.009 (4)	0.036 (3)
O3	0.215 (9)	0.108 (4)	0.093 (4)	0.054 (5)	0.044 (5)	-0.004 (3)
O4	0.128 (7)	0.259 (9)	0.104 (4)	-0.074 (7)	-0.041 (5)	0.035 (5)
N1	0.054 (4)	0.054 (3)	0.045 (3)	-0.005 (2)	0.001 (3)	-0.006 (3)
N2	0.047 (3)	0.056 (3)	0.047 (3)	0.004 (3)	0.005 (3)	-0.001 (2)
N3	0.051 (3)	0.056 (3)	0.058 (3)	-0.007 (3)	0.003 (3)	0.009 (3)
N4	0.043 (3)	0.067 (3)	0.049 (3)	0.006 (3)	-0.001 (2)	0.009 (2)
C1	0.065 (6)	0.077 (4)	0.058 (4)	0.002 (4)	-0.002 (4)	-0.004 (4)
C2	0.092 (7)	0.064 (4)	0.081 (5)	0.014 (5)	-0.005 (5)	-0.025 (4)
C3	0.076 (7)	0.055 (4)	0.099 (6)	0.010 (4)	-0.010 (5)	-0.011 (5)
C4	0.067 (6)	0.057 (4)	0.071 (4)	-0.002 (4)	-0.004 (4)	0.008 (4)
C5	0.044 (4)	0.038 (3)	0.062 (4)	-0.003 (3)	-0.007 (3)	-0.002 (3)
C6	0.043 (4)	0.050 (3)	0.049 (3)	-0.005 (3)	-0.003 (3)	0.005 (3)
C7	0.077 (6)	0.068 (4)	0.058 (4)	-0.015 (4)	-0.008 (4)	0.010 (4)
C8	0.070 (5)	0.101 (5)	0.047 (4)	-0.003 (5)	-0.001 (4)	0.006 (4)
C9	0.061 (5)	0.091 (5)	0.055 (4)	-0.013 (5)	0.008 (4)	-0.012 (4)
C10	0.056 (5)	0.064 (4)	0.060 (4)	0.001 (4)	0.001 (4)	-0.008 (3)
C11	0.054 (5)	0.068 (4)	0.075 (5)	0.000 (4)	0.002 (4)	0.001 (4)

C12	0.080 (7)	0.062 (4)	0.094 (6)	-0.015 (4)	0.017 (5)	0.007 (5)
C13	0.068 (6)	0.067 (4)	0.102 (6)	-0.008 (4)	0.014 (5)	-0.023 (5)
C14	0.068 (6)	0.067 (4)	0.075 (5)	-0.001 (4)	-0.002 (4)	-0.019 (4)
C15	0.048 (5)	0.051 (3)	0.062 (4)	0.002 (3)	-0.009 (3)	-0.009 (3)
C16	0.066 (5)	0.051 (4)	0.051 (4)	0.016 (4)	-0.017 (4)	0.003 (3)
C17	0.088 (6)	0.066 (4)	0.063 (4)	0.004 (4)	-0.018 (5)	-0.012 (4)
C18	0.122 (9)	0.084 (5)	0.049 (4)	0.002 (6)	-0.008 (5)	-0.005 (4)
C19	0.115 (8)	0.096 (6)	0.048 (4)	0.006 (6)	0.011 (4)	0.017 (4)
C20	0.079 (6)	0.097 (5)	0.060 (4)	-0.008 (5)	0.007 (4)	0.014 (4)

Geometric parameters (Å, °)

Fe1—N2	2.087 (4)	C5—C6	1.432 (8)
Fe1—N4	2.096 (5)	C6—C7	1.385 (8)
Fe1—N1	2.121 (5)	C7—C8	1.336 (9)
Fe1—N3	2.147 (5)	C7—H7	0.9300
Fe1—Cl3	2.2074 (18)	C8—C9	1.310 (9)
Fe1—Cl2	2.220 (2)	C8—H8	0.9300
Cl1—O2	1.363 (5)	C9—C10	1.366 (8)
Cl1—O4	1.366 (7)	C9—H9	0.9300
Cl1—O3	1.371 (5)	C10—H10	0.9300
Cl1—O1	1.373 (6)	C11—C12	1.346 (11)
N1—C1	1.302 (8)	C11—H11	0.9300
N1—C5	1.332 (7)	C12—C13	1.340 (11)
N2—C6	1.306 (7)	C12—H12	0.9300
N2—C10	1.324 (7)	C13—C14	1.346 (9)
N3—C11	1.306 (8)	C13—H13	0.9300
N3—C15	1.330 (7)	C14—C15	1.358 (9)
N4—C16	1.311 (8)	C14—H14	0.9300
N4—C20	1.329 (8)	C15—C16	1.444 (9)
C1—C2	1.360 (10)	C16—C17	1.365 (8)
C1—H1	0.9300	C17—C18	1.353 (10)
C2—C3	1.362 (10)	C17—H17	0.9300
C2—H2	0.9300	C18—C19	1.344 (11)
C3—C4	1.342 (9)	C18—H18	0.9300
C3—H3	0.9300	C19—C20	1.378 (9)
C4—C5	1.350 (9)	C19—H19	0.9300
C4—H4	0.9300	C20—H20	0.9300
N2—Fe1—N4	160.23 (18)	C4—C5—C6	123.6 (6)
N2—Fe1—N1	75.96 (19)	N2—C6—C7	119.5 (6)
N4—Fe1—N1	90.98 (18)	N2—C6—C5	116.0 (5)
N2—Fe1—N3	88.34 (19)	C7—C6—C5	124.5 (6)
N4—Fe1—N3	75.4 (2)	C8—C7—C6	120.7 (7)
N1—Fe1—N3	84.2 (2)	C8—C7—H7	119.6
N2—Fe1—Cl3	97.95 (16)	C6—C7—H7	119.6
N4—Fe1—Cl3	93.40 (14)	C9—C8—C7	119.1 (7)
N1—Fe1—Cl3	171.80 (16)	C9—C8—H8	120.5
N3—Fe1—Cl3	90.20 (15)	C7—C8—H8	120.5
N2—Fe1—Cl2	94.29 (15)	C8—C9—C10	119.7 (7)

supplementary materials

N4—Fe1—C12	99.84 (16)	C8—C9—H9	120.1
N1—Fe1—C12	86.93 (15)	C10—C9—H9	120.1
N3—Fe1—C12	169.85 (15)	N2—C10—C9	121.6 (6)
C13—Fe1—C12	99.13 (8)	N2—C10—H10	119.2
O2—C11—O4	109.4 (5)	C9—C10—H10	119.2
O2—C11—O3	108.0 (4)	N3—C11—C12	124.8 (7)
O4—C11—O3	111.0 (6)	N3—C11—H11	117.6
O2—C11—O1	110.7 (4)	C12—C11—H11	117.6
O4—C11—O1	106.7 (4)	C13—C12—C11	117.1 (8)
O3—C11—O1	111.0 (4)	C13—C12—H12	121.4
C1—N1—C5	119.5 (6)	C11—C12—H12	121.4
C1—N1—Fe1	125.7 (4)	C12—C13—C14	119.8 (8)
C5—N1—Fe1	114.8 (4)	C12—C13—H13	120.1
C6—N2—C10	119.3 (5)	C14—C13—H13	120.1
C6—N2—Fe1	117.1 (4)	C13—C14—C15	120.2 (7)
C10—N2—Fe1	123.5 (4)	C13—C14—H14	119.9
C11—N3—C15	117.8 (6)	C15—C14—H14	119.9
C11—N3—Fe1	127.5 (5)	N3—C15—C14	120.2 (7)
C15—N3—Fe1	114.6 (4)	N3—C15—C16	116.3 (6)
C16—N4—C20	119.2 (6)	C14—C15—C16	123.5 (6)
C16—N4—Fe1	117.6 (4)	N4—C16—C17	121.7 (7)
C20—N4—Fe1	123.0 (5)	N4—C16—C15	115.4 (5)
N1—C1—C2	122.8 (7)	C17—C16—C15	122.9 (7)
N1—C1—H1	118.6	C18—C17—C16	119.2 (7)
C2—C1—H1	118.6	C18—C17—H17	120.4
C1—C2—C3	117.5 (7)	C16—C17—H17	120.4
C1—C2—H2	121.3	C19—C18—C17	120.0 (7)
C3—C2—H2	121.3	C19—C18—H18	120.0
C4—C3—C2	119.7 (7)	C17—C18—H18	120.0
C4—C3—H3	120.1	C18—C19—C20	118.4 (8)
C2—C3—H3	120.1	C18—C19—H19	120.8
C3—C4—C5	120.1 (7)	C20—C19—H19	120.8
C3—C4—H4	119.9	N4—C20—C19	121.6 (8)
C5—C4—H4	119.9	N4—C20—H20	119.2
N1—C5—C4	120.3 (6)	C19—C20—H20	119.2
N1—C5—C6	116.1 (5)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg4 is the centroid of the N2,C6–C10 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3 \cdots O2	0.93	2.52	3.140 (11)	124
C7—H7 \cdots O3 ⁱ	0.93	2.55	3.239 (9)	131
C8—H8 \cdots O2 ⁱⁱ	0.93	2.30	3.152 (9)	152
C13—H13 \cdots O2 ⁱⁱⁱ	0.93	2.54	3.423 (10)	158
C18—H18 \cdots O4 ^{iv}	0.93	2.51	3.387 (10)	158
C10—H10 \cdots C13	0.93	2.71	3.308 (7)	122
C20—H20 \cdots C12	0.93	2.79	3.382 (7)	123

C11—H11 \cdots Cg4

0.93

2.90

3.705 (8)

146

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

Fig. 1

