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2-Amino-4-(4-bromophenyl)-6-ferrocenylpyridine-3-carbonitrile

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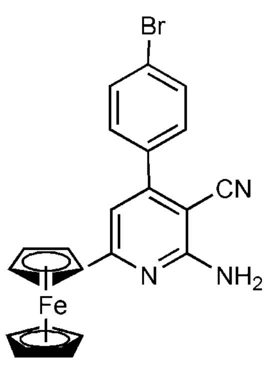
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.038; wR factor = 0.094; data-to-parameter ratio = 13.5.

The title compound, $[Fe(C_5H_5)(C_{17}H_{11}BrN_3)]$, was synthesized by the reaction of 4-bromobenzaldehyde, acetylferrocene and ammonium acetate in an aqueous medium. The crystal packing is stabilized by intermolecular N—H···N hydrogen bonds. The dihedral angles between the phenyl ring and the pyridine and cyclopentadienyl rings are 51.67 (13) and 12.12 (21)°, respectively.

Related literature

For related literature, see: Alyoubi (2000); Desai & Shah (2003); Dombrowski *et al.* (1986); Murata *et al.* (2004).



Experimental

Crystal data

$[Fe(C_5H_5)(C_{17}H_{11}BrN_3)]$
M_r = 458.14
Monoclinic, $P2_1/n$
a = 12.250 (2) Å
b = 7.4511 (12) Å
c = 20.698 (3) Å
β = 97.729 (3)°
V = 1872.2 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.95 mm^{-1}
T = 298 (2) K
0.16 × 0.11 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.650, T_{max} = 0.820
9276 measured reflections
3290 independent reflections
2327 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.094
S = 1.02
3290 reflections
244 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N3^{i}	0.86	2.29	3.050 (5)	148

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); 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: BQ2041).

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supporting information

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2-Amino-4-(4-bromophenyl)-6-ferrocenylpyridine-3-carbonitrile

Run-Hong Jia and Shu-Jiang Tu

S1. Comment

Metallocenes are known to exhibit a wide range of biological activity. Among them, ferrocene has attracted special attention since it is neutral, chemically stable, non-toxic and able to cross cell membranes (Dombrowski *et al.*, 1986). In fact, it is now well established that the incorporation of ferrocene units in organic molecules introduces significant and new properties in these materials. In addition, it has been demonstrated that molecules containing cyanopyridine moiety may be able to work as ligands towards transition-metal ions (Alyoubi, 2000), new drugs (Murata *et al.*, 2004 and Desai *et al.*, 2003), and significant intermediates for the synthesis of important vitamins such as nicotinic acids and nicotinamides. For these reasons, the synthesis of new compounds containing cyanopyridine derivatives is strongly desired. In this paper we report the crystal structure of the title compound (I).

In the crystal structure, the dihedral angle between the C1/C2/C3/C4/C5/N1 plane and the C17—C22 benzene ring is 51.65 (13)°.The dihedral angle between the C1/C2/C3/C4/C5/N1 plane and the C11—C16 ring is 12.21 (14)°. The molecules are connected *via* N—H···N hydrogen bonds, forming a three-dimensional network (Fig. 2).

S2. Experimental

Compound (I) was prepared by the reaction of 4-bromobenzaldehyde (2 mmol), malononitrile (2 mmol), acetylferrocene (2 mmol) and ammonium acetate (4 mmol) in water (2 ml). Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 94%; m.p. >573 K). IR (cm^{-1}): 3457, 3354, 2211; ^{1}H NMR (DMSO-d_6): 4.10 (5*H*, s, ferrocenyl), 4.50 (2*H*, s, ferrocenyl), 5.04 (2*H*, s, ferrocenyl), 6.83 (2*H*, brs, NH_2), 6.94 (1*H*, s, ArH), 7.60 (2*H*, d, J = 8.0 Hz, ArH), 7.77 (2*H*, d, J = 8.0 Hz, ArH).7.87 (2*H*, brs, NH_2), 7.88–8.01 (4*H*, m, ArH), 11.85 (1*H*, s, NH).

S3. Refinement

All H atoms were positioned geometrically and treated as riding, with N—H = 0.86 Å and C—H = 0.93–0.97 Å.

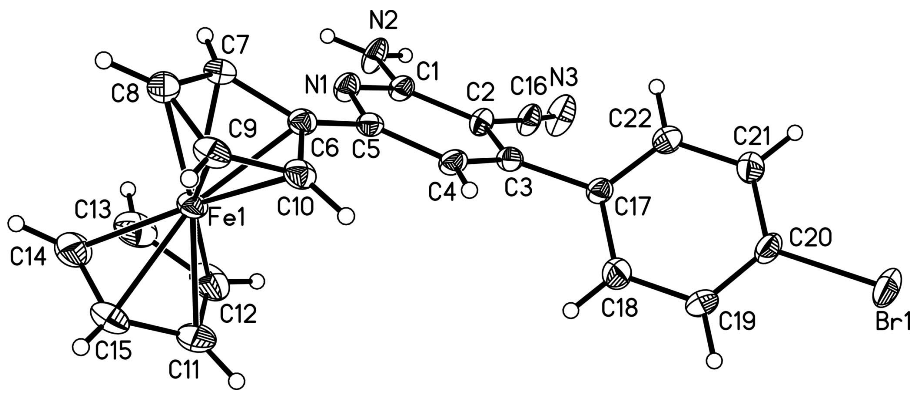

Figure 1

The molecular structure of title compound, showing 30% probability displacement ellipsoids.

2-Amino-4-(4-bromophenyl)-6-ferrocenylpyridine-3-carbonitrile

Crystal data

$[Fe(C_5H_5)(C_{17}H_{11}BrN_3)]$
$M_r = 458.14$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 12.250$ (2) Å
$b = 7.4511$ (12) Å
$c = 20.698$ (3) Å
$\beta = 97.729$ (3)°
$V = 1872.2$ (5) Å^3
$Z = 4$
$F(000) = 920$
$D_x = 1.625$ Mg m^{-3}
Melting point > 573 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9276 reflections
$\theta = 1.8$–25.0°
$\mu = 2.95$ mm^{-1}
$T = 298$ K
Block, red
0.16 × 0.11 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.650$, $T_{max} = 0.820$
9276 measured reflections
3290 independent reflections
2327 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
$h = -14 \rightarrow 12$
$k = -8 \rightarrow 8$
$l = -21 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.094$
$S = 1.02$
3290 reflections
244 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
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 0.873P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ 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 $F^2 > \sigma(F^2)$ 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	0.88176 (4)	0.56744 (7)	0.10748 (3)	0.03294 (17)
Br1	1.31762 (4)	−0.46355 (6)	0.38737 (3)	0.06095 (19)
N1	0.8559 (2)	0.4500 (4)	0.27746 (15)	0.0335 (7)
N2	0.8621 (3)	0.5510 (4)	0.38201 (16)	0.0441 (9)
H2A	0.8136	0.6301	0.3678	0.053*
H2B	0.8871	0.5466	0.4228	0.053*
N3	1.0484 (3)	0.3011 (5)	0.48388 (19)	0.0596 (11)
C1	0.8991 (3)	0.4337 (5)	0.34017 (18)	0.0319 (9)
C2	0.9785 (3)	0.3014 (5)	0.36174 (18)	0.0302 (8)
C3	1.0146 (3)	0.1847 (5)	0.31590 (18)	0.0302 (9)
C4	0.9720 (3)	0.2070 (5)	0.25112 (18)	0.0313 (9)
H4	0.9956	0.1339	0.2193	0.038*
C5	0.8928 (3)	0.3408 (5)	0.23362 (17)	0.0274 (8)
C6	0.8419 (3)	0.3651 (5)	0.16587 (17)	0.0295 (8)
C7	0.7494 (3)	0.4767 (5)	0.14559 (18)	0.0328 (9)
H7	0.7103	0.5424	0.1731	0.039*
C8	0.7267 (3)	0.4714 (5)	0.0769 (2)	0.0404 (10)
H8	0.6696	0.5310	0.0514	0.048*
C9	0.8063 (3)	0.3594 (5)	0.05372 (19)	0.0384 (9)
H9	0.8107	0.3334	0.0102	0.046*
C10	0.8781 (3)	0.2935 (5)	0.10802 (18)	0.0343 (9)
H10	0.9379	0.2175	0.1064	0.041*
C11	1.0377 (4)	0.6526 (6)	0.1005 (2)	0.0542 (12)
H11	1.0979	0.5798	0.0960	0.065*
C12	1.0040 (4)	0.7097 (6)	0.1601 (3)	0.0596 (13)
H12	1.0381	0.6819	0.2018	0.072*
C13	0.9095 (4)	0.8163 (6)	0.1444 (3)	0.0597 (13)
H13	0.8697	0.8711	0.1741	0.072*
C14	0.8852 (4)	0.8261 (6)	0.0762 (3)	0.0586 (13)
H14	0.8269	0.8885	0.0530	0.070*
C15	0.9639 (4)	0.7257 (6)	0.0495 (2)	0.0533 (12)
H15	0.9671	0.7098	0.0053	0.064*
C16	1.0201 (3)	0.2954 (5)	0.4291 (2)	0.0395 (10)
C17	1.0911 (3)	0.0326 (5)	0.33629 (17)	0.0306 (8)
C18	1.1829 (3)	0.0036 (5)	0.3047 (2)	0.0439 (10)

H18	1.1986	0.0831	0.2725	0.053*
C19	1.2509 (3)	−0.1418 (6)	0.3206 (2)	0.0461 (11)
H19	1.3125	−0.1601	0.2996	0.055*
C20	1.2267 (3)	−0.2594 (5)	0.3678 (2)	0.0389 (10)
C21	1.1376 (3)	−0.2323 (5)	0.3997 (2)	0.0484 (11)
H21	1.1226	−0.3120	0.4320	0.058*
C22	1.0702 (3)	−0.0868 (5)	0.3841 (2)	0.0455 (11)
H22	1.0097	−0.0686	0.4060	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0303 (3)	0.0277 (3)	0.0417 (3)	−0.0076 (2)	0.0078 (2)	0.0011 (2)
Br1	0.0584 (3)	0.0489 (3)	0.0780 (4)	0.0306 (2)	0.0181 (3)	0.0102 (3)
N1	0.0335 (18)	0.0312 (17)	0.0363 (18)	0.0084 (14)	0.0065 (14)	−0.0016 (15)
N2	0.048 (2)	0.045 (2)	0.0387 (19)	0.0278 (17)	0.0043 (16)	−0.0063 (16)
N3	0.070 (3)	0.065 (3)	0.041 (2)	0.031 (2)	−0.002 (2)	−0.005 (2)
C1	0.028 (2)	0.030 (2)	0.038 (2)	0.0045 (16)	0.0073 (17)	−0.0006 (18)
C2	0.030 (2)	0.0270 (19)	0.033 (2)	0.0053 (16)	0.0019 (16)	−0.0024 (16)
C3	0.027 (2)	0.0275 (19)	0.037 (2)	−0.0008 (16)	0.0081 (17)	0.0005 (17)
C4	0.027 (2)	0.0300 (19)	0.039 (2)	0.0041 (16)	0.0100 (17)	−0.0031 (17)
C5	0.026 (2)	0.0267 (19)	0.031 (2)	−0.0012 (15)	0.0091 (16)	−0.0010 (16)
C6	0.028 (2)	0.0263 (18)	0.035 (2)	−0.0034 (16)	0.0058 (16)	−0.0018 (17)
C7	0.029 (2)	0.035 (2)	0.036 (2)	−0.0065 (17)	0.0084 (16)	−0.0015 (17)
C8	0.033 (2)	0.040 (2)	0.048 (3)	−0.0059 (18)	0.0007 (18)	0.005 (2)
C9	0.041 (2)	0.041 (2)	0.034 (2)	−0.013 (2)	0.0084 (18)	−0.0028 (19)
C10	0.037 (2)	0.0253 (19)	0.042 (2)	−0.0050 (17)	0.0114 (18)	−0.0030 (18)
C11	0.036 (3)	0.052 (3)	0.075 (4)	−0.018 (2)	0.012 (2)	0.008 (3)
C12	0.060 (3)	0.052 (3)	0.064 (3)	−0.035 (3)	−0.005 (3)	0.003 (2)
C13	0.067 (4)	0.035 (2)	0.080 (4)	−0.021 (2)	0.023 (3)	−0.012 (3)
C14	0.055 (3)	0.035 (2)	0.088 (4)	−0.006 (2)	0.020 (3)	0.011 (3)
C15	0.053 (3)	0.050 (3)	0.059 (3)	−0.017 (2)	0.020 (2)	0.011 (2)
C16	0.042 (3)	0.037 (2)	0.039 (3)	0.0170 (19)	0.006 (2)	−0.0008 (19)
C17	0.028 (2)	0.0270 (19)	0.037 (2)	0.0028 (16)	0.0087 (16)	−0.0027 (17)
C18	0.048 (3)	0.038 (2)	0.049 (3)	0.0091 (19)	0.018 (2)	0.006 (2)
C19	0.038 (2)	0.047 (2)	0.058 (3)	0.011 (2)	0.024 (2)	0.003 (2)
C20	0.033 (2)	0.032 (2)	0.052 (3)	0.0118 (17)	0.0080 (19)	−0.003 (2)
C21	0.050 (3)	0.039 (2)	0.061 (3)	0.012 (2)	0.023 (2)	0.013 (2)
C22	0.040 (2)	0.042 (2)	0.059 (3)	0.012 (2)	0.024 (2)	0.007 (2)

Geometric parameters (Å, º)

Fe1—C7	2.013 (4)	C7—C8	1.412 (5)
Fe1—C13	2.017 (4)	C7—H7	0.9300
Fe1—C12	2.028 (4)	C8—C9	1.416 (5)
Fe1—C6	2.033 (4)	C8—H8	0.9300
Fe1—C14	2.035 (4)	C9—C10	1.419 (5)
Fe1—C11	2.037 (4)	C9—H9	0.9300

Fe1—C15	2.041 (4)	C10—H10	0.9300
Fe1—C10	2.042 (4)	C11—C15	1.404 (6)
Fe1—C8	2.049 (4)	C11—C12	1.417 (6)
Fe1—C9	2.054 (4)	C11—H11	0.9300
Br1—C20	1.897 (4)	C12—C13	1.406 (6)
N1—C1	1.340 (5)	C12—H12	0.9300
N1—C5	1.342 (4)	C13—C14	1.404 (7)
N2—C1	1.351 (4)	C13—H13	0.9300
N2—H2A	0.8600	C14—C15	1.392 (6)
N2—H2B	0.8600	C14—H14	0.9300
N3—C16	1.140 (5)	C15—H15	0.9300
C1—C2	1.415 (5)	C17—C22	1.380 (5)
C2—C3	1.402 (5)	C17—C18	1.392 (5)
C2—C16	1.420 (6)	C18—C19	1.379 (5)
C3—C4	1.382 (5)	C18—H18	0.9300
C3—C17	1.495 (5)	C19—C20	1.374 (5)
C4—C5	1.404 (5)	C19—H19	0.9300
C4—H4	0.9300	C20—C21	1.365 (5)
C5—C6	1.468 (5)	C21—C22	1.375 (5)
C6—C7	1.423 (5)	C21—H21	0.9300
C6—C10	1.435 (5)	C22—H22	0.9300

C7—Fe1—C13	105.30 (18)	C6—C7—Fe1	70.1 (2)
C7—Fe1—C12	122.73 (18)	C8—C7—H7	125.6
C13—Fe1—C12	40.67 (19)	C6—C7—H7	125.6
C7—Fe1—C6	41.17 (14)	Fe1—C7—H7	124.8
C13—Fe1—C6	119.91 (18)	C7—C8—C9	107.8 (3)
C12—Fe1—C6	106.72 (17)	C7—C8—Fe1	68.3 (2)
C7—Fe1—C14	119.64 (17)	C9—C8—Fe1	70.0 (2)
C13—Fe1—C14	40.54 (18)	C7—C8—H8	126.1
C12—Fe1—C14	68.3 (2)	C9—C8—H8	126.1
C6—Fe1—C14	155.28 (18)	Fe1—C8—H8	127.2
C7—Fe1—C11	160.93 (17)	C8—C9—C10	108.5 (3)
C13—Fe1—C11	68.2 (2)	C8—C9—Fe1	69.6 (2)
C12—Fe1—C11	40.81 (18)	C10—C9—Fe1	69.3 (2)
C6—Fe1—C11	125.17 (17)	C8—C9—H9	125.7
C14—Fe1—C11	67.84 (19)	C10—C9—H9	125.7
C7—Fe1—C15	155.64 (17)	Fe1—C9—H9	127.0
C13—Fe1—C15	67.7 (2)	C9—C10—C6	107.7 (3)
C12—Fe1—C15	68.07 (19)	C9—C10—Fe1	70.2 (2)
C6—Fe1—C15	162.71 (17)	C6—C10—Fe1	69.1 (2)
C14—Fe1—C15	39.94 (17)	C9—C10—H10	126.1
C11—Fe1—C15	40.27 (17)	C6—C10—H10	126.1
C7—Fe1—C10	69.07 (15)	Fe1—C10—H10	126.2
C13—Fe1—C10	156.9 (2)	C15—C11—C12	107.7 (5)
C12—Fe1—C10	122.33 (18)	C15—C11—Fe1	70.1 (2)
C6—Fe1—C10	41.23 (14)	C12—C11—Fe1	69.3 (2)
C14—Fe1—C10	161.78 (19)	C15—C11—H11	126.2

C11—Fe1—C10	109.48 (18)	C12—C11—H11	126.2
C15—Fe1—C10	126.43 (17)	Fe1—C11—H11	126.1
C7—Fe1—C8	40.67 (15)	C13—C12—C11	107.2 (4)
C13—Fe1—C8	122.68 (19)	C13—C12—Fe1	69.2 (2)
C12—Fe1—C8	159.3 (2)	C11—C12—Fe1	69.9 (2)
C6—Fe1—C8	68.75 (15)	C13—C12—H12	126.4
C14—Fe1—C8	106.87 (18)	C11—C12—H12	126.4
C11—Fe1—C8	157.92 (18)	Fe1—C12—H12	126.0
C15—Fe1—C8	122.02 (18)	C14—C13—C12	108.6 (5)
C10—Fe1—C8	68.44 (16)	C14—C13—Fe1	70.4 (3)
C7—Fe1—C9	68.36 (15)	C12—C13—Fe1	70.1 (2)
C13—Fe1—C9	160.0 (2)	C14—C13—H13	125.7
C12—Fe1—C9	158.7 (2)	C12—C13—H13	125.7
C6—Fe1—C9	68.62 (15)	Fe1—C13—H13	125.3
C14—Fe1—C9	124.71 (19)	C15—C14—C13	107.8 (5)
C11—Fe1—C9	123.72 (18)	C15—C14—Fe1	70.3 (2)
C15—Fe1—C9	109.84 (17)	C13—C14—Fe1	69.0 (3)
C10—Fe1—C9	40.53 (14)	C15—C14—H14	126.1
C8—Fe1—C9	40.36 (15)	C13—C14—H14	126.1
C1—N1—C5	118.3 (3)	Fe1—C14—H14	126.2
C1—N2—H2A	120.0	C14—C15—C11	108.7 (4)
C1—N2—H2B	120.0	C14—C15—Fe1	69.8 (2)
H2A—N2—H2B	120.0	C11—C15—Fe1	69.7 (2)
N1—C1—N2	116.1 (3)	C14—C15—H15	125.6
N1—C1—C2	122.3 (3)	C11—C15—H15	125.6
N2—C1—C2	121.6 (3)	Fe1—C15—H15	126.5
C3—C2—C1	119.0 (3)	N3—C16—C2	174.9 (4)
C3—C2—C16	122.8 (3)	C22—C17—C18	118.5 (3)
C1—C2—C16	118.2 (3)	C22—C17—C3	121.4 (3)
C4—C3—C2	118.0 (3)	C18—C17—C3	120.0 (3)
C4—C3—C17	120.4 (3)	C19—C18—C17	120.7 (4)
C2—C3—C17	121.5 (3)	C19—C18—H18	119.7
C3—C4—C5	119.6 (3)	C17—C18—H18	119.7
C3—C4—H4	120.2	C20—C19—C18	119.3 (4)
C5—C4—H4	120.2	C20—C19—H19	120.4
N1—C5—C4	122.7 (3)	C18—C19—H19	120.4
N1—C5—C6	115.6 (3)	C21—C20—C19	120.9 (4)
C4—C5—C6	121.6 (3)	C21—C20—Br1	120.0 (3)
C7—C6—C10	107.1 (3)	C19—C20—Br1	119.1 (3)
C7—C6—C5	125.0 (3)	C20—C21—C22	119.8 (4)
C10—C6—C5	127.7 (3)	C20—C21—H21	120.1
C7—C6—Fe1	68.7 (2)	C22—C21—H21	120.1
C10—C6—Fe1	69.7 (2)	C21—C22—C17	120.9 (4)
C5—C6—Fe1	123.7 (2)	C21—C22—H22	119.5
C8—C7—C6	108.8 (3)	C17—C22—H22	119.5
C8—C7—Fe1	71.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···N3^{i}	0.86	2.29	3.050 (5)	148

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