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1-Ferrocenyl-3-(4-methylanilino)propan-1-one

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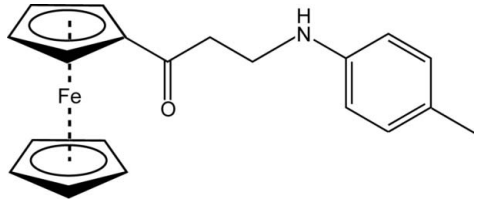
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.115; data-to-parameter ratio = 16.5.

In the title ferrocene derivative, $[Fe(C_5H_5)(C_{15}H_{16}NO)]$, the dihedral angle between the best planes of the benzene and the substituted cyclopentadienyl ring is 83.4 (1)°. The presence of a methyl substituent in the *para* position of the aniline group does not alter the crystal packing compared to that of 3-anilino-1-ferrocenylpropan-1-one [Leka *et al.* (2012). *Acta Cryst.* E**68**, m229]. The molecules are connected into centrosymmetric dimers *via* N—H···O hydrogen bonds. In addition, C—H···O and C—H···N contacts stabilize the crystal packing.

Related literature

For the physico-chemical properties of ferrocene-based compounds, see: Togni & Hayashi (1995). For related crystal structures and details of the synthesis, see: Damljanović *et al.* (2011); Stevanović *et al.* (2012); Leka *et al.* (2012*a*,*b*).



Experimental

Crystal data

$[Fe(C_5H_5)(C_{15}H_{16}NO)]$
M_r = 347.23
Triclinic, $P\overline{1}$
a = 7.553 (2) Å
b = 9.778 (3) Å
c = 13.640 (4) Å
α = 86.83 (2)°
β = 74.62 (3)°
γ = 67.71 (3)°
V = 897.6 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.84 mm^{-1}
T = 293 K
0.22 × 0.18 × 0.16 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
3804 measured reflections
3519 independent reflections
2829 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
3 standard reflections every 60 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
S = 1.05
3519 reflections
213 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O1^{i}	0.82 (3)	2.31 (4)	3.102 (4)	161 (3)
C19—H19···O1^{i}	0.93	2.69	3.455 (4)	140
C4—H4···N1^{ii}	0.93	2.64	3.451 (4)	147

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x+1, y-1, z$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *POV-RAY* (Persistence of Vision, 2004); software used to prepare material for publication: *WinGX* (Farrugia, 1999), *PLATON* (Spek, 2009) and *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5791).

References

Damljanović, I., Stevanović, D., Pejović, A., Vukićević, M., Novaković, S. B., Bogdanović, G. A., Mihajlov-Krstev, T., Radulović, N. & Vukićević, R. D. (2011). *J. Organomet. Chem.* **696**, 3703–3713.
Enraf–Nonius (1989). *CAD-4 Software*. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Leka, Z., Novaković, S. B., Stevanović, D., Bogdanović, G. A. & Vukićević, R. D. (2012*a*). *Acta Cryst.* E**68**, m229.
Leka, Z., Novaković, S. B., Stevanović, D., Bogdanović, G. A. & Vukićević, R. D. (2012*b*). *Acta Cryst.* E**68**, m231.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Persistence of Vision (2004). *POV-RAY*. Persistence of Vision Pty Ltd, Williamstown, Victoria, Australia. URL: http://www.povray.org/.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Stevanović, D., Pejović, A., Novaković, S. B., Bogdanović, G. A., Divjaković, V. & Vukićević, R. D. (2012). *Acta Cryst.* C**68**, m37–m40.
Togni, A. & Hayashi, T. (1995). *Ferrocenes: Homogeneous Catalysis, Organic Synthesis, Materials Science*. New York: VCH.

supporting information

Acta Cryst. (2012). E**68**, m230 [doi:10.1107/S1600536812003509]

1-Ferrocenyl-3-(4-methylanilino)propan-1-one

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S1. Comment

The present report forms a part of our wider research of the structural properties of Mannich bases. The title compound (Figure 1) crystallizes in the same space group, *i.e.* $P\bar{1}$, as the derivative containing an unsubstitued phenylamino moiety and exhibits very similar unit-cell parameters. The orientation of the cyclopentadienyl (Cp) rings slightly deviates from the eclipsed conformation as defined by the smallest torsion angle C—C*g*1—C*g*2—C of 4.9° (*Cg*1 and *Cg*2 are centroids of the corresponding Cp rings). The distances of Fe to C*g*1 and C*g*2 are 1.65 and 1.66°, respectively. The Cp rings are practically coplanar with the dihedral angle of 0.5 (2)°. The torsion angle O1—C11—C1—C5 which relates Cp1 ring with the carbonyl group is here equal to -6.2 (3)°, showing the expected co-planarity. Although C1—C11—C12—C13—N1 fragment consists of single bonds which allows for free rotation, the molecule adopts a conformation very similar to the previously reported derivatives (Damljanović *et al.*, 2011; Stevanović *et al.*, 2012). The bent conformation of the molecule is indicated by the C11—C12—C13— N1 torsion angle [(70.6 (3)°] which is slightly smaller than in the case of the molecule containing unmodified, phenylamino moiety. Regardless the fact that molecules of the present Mannich base contain an additional methyl subsistent in the *para* position of the phenylamino moiety their crystal packing arrangement (Figure 2) is closely similar to the previously reported 1-ferrocenyl-3-(phenylamino)propan-1-one (Leka *et al*., 2012*a*). As previously observed, the N—H···O bonded dimers represent the main structural feature of these Mannich basis. The methyl group does not take a part in the intermolecular interactions.

S2. Experimental

The compound was obtained in the reaction of aza-Michael addition of corresponding arylamine to acryloylferrocene. The reaction was performed by microwave (MW) irradiation (500 W/5 min) of a mixture of reactants and montmorillonite K-10, without a solvent as described by Damljanović *et al.* (2011).

S3. Refinement

H atoms bonded to C atoms were placed at geometrically calculated positions and refined using a riding model. C—H distances were fixed to 0.93, 0.97 and 0.96 Å from aromatic, methylene and methyl C atoms, respectively. The U_{iso}(H) values were equal to 1.2 times U_{eq} of the corresponding aromatic C(sp^2) and methylene C(sp^3). The U_{iso}(H) values of the H atoms attached to methyl C(sp^3) were equal to 1.5 times U_{eq} of the parent atom. H atom attached to N atom was refined isotropically.

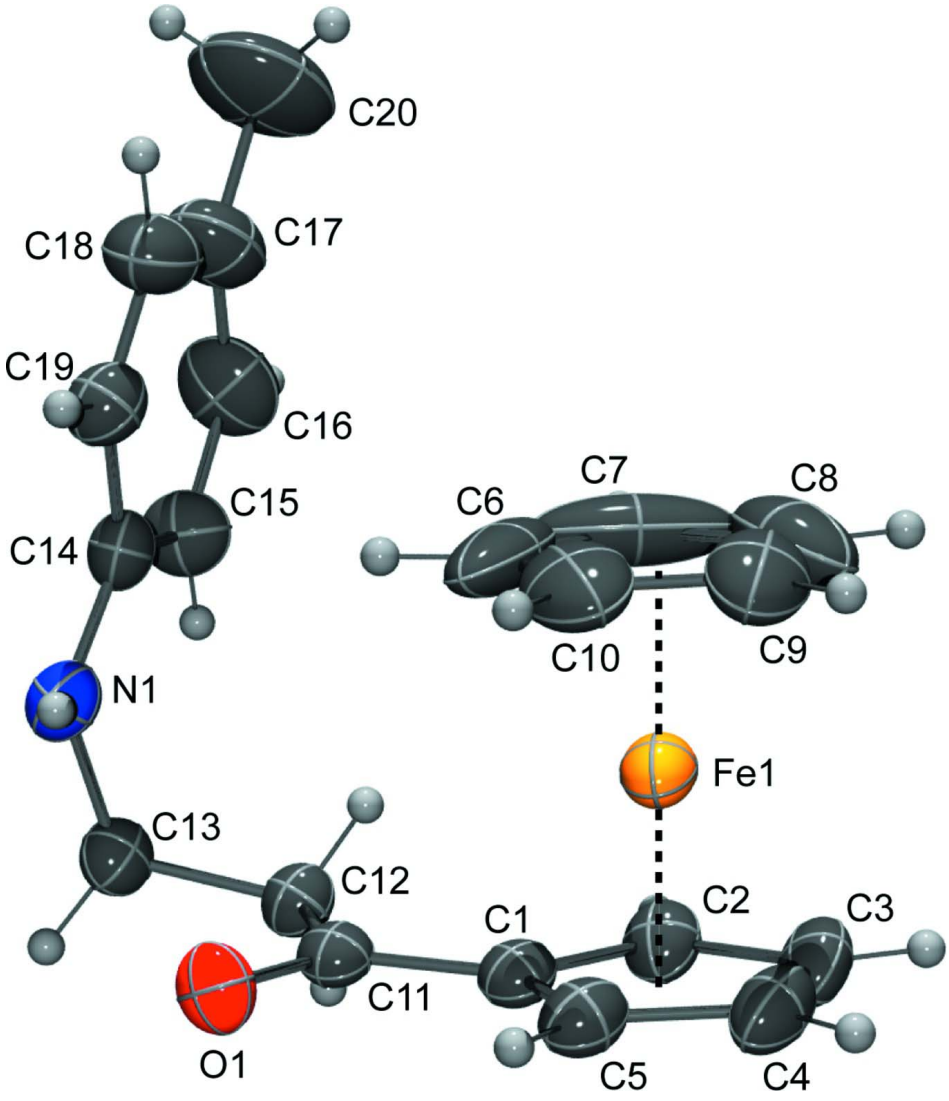

Figure 1

The molecular structure of the title compound, with atom labels and 40% probability displacement ellipsoids for non-H atoms.

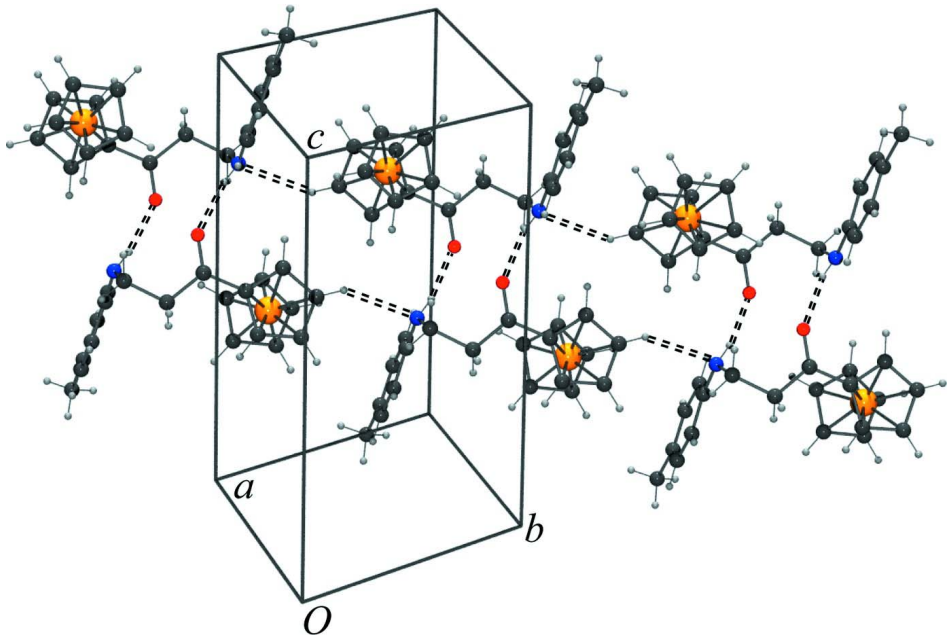

Figure 2

Part of the crystal packing showing the interconnection of dimers into a chain.

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Crystal data

$[Fe(C_5H_5)(C_{15}H_{16}NO)]$
$M_r = 347.23$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.553$ (2) Å
$b = 9.778$ (3) Å
$c = 13.640$ (4) Å
$\alpha = 86.83$ (2)°
$\beta = 74.62$ (3)°
$\gamma = 67.71$ (3)°
$V = 897.6$ (5) Å^3
$Z = 2$
$F(000) = 364$
$D_x = 1.285$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 11.2$–15.5°
$\mu = 0.84$ mm^{-1}
$T = 293$ K
Prismatic, orange
0.22 × 0.18 × 0.16 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
3804 measured reflections
3519 independent reflections
2829 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.6°$
$h = 0 \rightarrow 9$
$k = -11 \rightarrow 12$
$l = -16 \rightarrow 16$
3 standard reflections every 60 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.115$
$S = 1.05$
3519 reflections
213 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.2205P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.82439 (5)	−0.29783 (4)	0.68484 (3)	0.04989 (14)
O1	0.7296 (3)	−0.01261 (19)	0.48727 (13)	0.0550 (4)
N1	0.3609 (3)	0.2268 (2)	0.63329 (17)	0.0487 (5)
C1	0.9228 (3)	−0.1577 (2)	0.59236 (17)	0.0434 (5)
C2	1.0021 (4)	−0.1826 (3)	0.6791 (2)	0.0522 (6)
H2	0.9830	−0.1105	0.7269	0.063*
C3	1.1144 (4)	−0.3355 (3)	0.6796 (2)	0.0626 (7)
H3	1.1817	−0.3814	0.7278	0.075*
C4	1.1072 (4)	−0.4068 (3)	0.5945 (2)	0.0619 (7)
H4	1.1689	−0.5076	0.5771	0.074*
C5	0.9901 (4)	−0.2987 (3)	0.5400 (2)	0.0525 (6)
H5	0.9617	−0.3161	0.4807	0.063*
C6	0.5242 (5)	−0.2197 (5)	0.7206 (5)	0.119 (2)
H6	0.4437	−0.1340	0.6968	0.142*
C7	0.5913 (10)	−0.2274 (8)	0.8092 (5)	0.154 (3)
H7	0.5661	−0.1504	0.8545	0.185*
C8	0.7072 (8)	−0.3819 (7)	0.8128 (3)	0.1120 (17)
H8	0.7720	−0.4250	0.8625	0.134*
C9	0.7059 (5)	−0.4533 (4)	0.7321 (3)	0.0885 (11)
H9	0.7712	−0.5546	0.7169	0.106*
C10	0.5963 (5)	−0.3570 (5)	0.6763 (3)	0.0930 (12)
H10	0.5739	−0.3812	0.6169	0.112*
C11	0.7851 (3)	−0.0189 (2)	0.56467 (17)	0.0416 (5)
C12	0.7182 (3)	0.1184 (2)	0.63237 (18)	0.0452 (5)
H12B	0.8298	0.1477	0.6260	0.054*
H12A	0.6756	0.0955	0.7027	0.054*
C13	0.5489 (4)	0.2475 (3)	0.6063 (2)	0.0497 (5)
H13B	0.5316	0.3370	0.6416	0.060*
H13A	0.5848	0.2613	0.5337	0.060*
C14	0.2552 (4)	0.2300 (3)	0.73370 (19)	0.0466 (5)
C15	0.2798 (5)	0.2977 (3)	0.8142 (2)	0.0643 (7)
H15	0.3764	0.3382	0.8020	0.077*
C16	0.1612 (6)	0.3046 (4)	0.9115 (2)	0.0861 (10)
H16	0.1805	0.3503	0.9636	0.103*
C17	0.0152 (6)	0.2468 (4)	0.9352 (3)	0.0878 (10)
C18	−0.0069 (5)	0.1779 (4)	0.8545 (3)	0.0789 (9)
H18	−0.1029	0.1367	0.8673	0.095*
C19	0.1089 (4)	0.1693 (3)	0.7571 (2)	0.0575 (6)

H19	0.0901	0.1223	0.7055	0.069*
C20	−0.1148 (9)	0.2559 (7)	1.0428 (3)	0.154 (2)
H20A	−0.0632	0.2899	1.0895	0.230*
H20B	−0.1157	0.1597	1.0605	0.230*
H20C	−0.2477	0.3237	1.0464	0.230*
H1N	0.366 (4)	0.163 (3)	0.595 (2)	0.047 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0419 (2)	0.0508 (2)	0.0630 (2)	−0.02310 (15)	−0.01730 (16)	0.01293 (16)
O1	0.0657 (11)	0.0563 (10)	0.0499 (9)	−0.0244 (9)	−0.0245 (8)	0.0024 (8)
N1	0.0461 (11)	0.0494 (11)	0.0521 (12)	−0.0159 (9)	−0.0168 (9)	−0.0059 (9)
C1	0.0377 (11)	0.0467 (12)	0.0505 (12)	−0.0219 (9)	−0.0105 (9)	0.0024 (10)
C2	0.0483 (13)	0.0542 (14)	0.0653 (15)	−0.0255 (11)	−0.0246 (12)	0.0070 (12)
C3	0.0440 (13)	0.0614 (16)	0.090 (2)	−0.0211 (12)	−0.0318 (13)	0.0194 (14)
C4	0.0434 (13)	0.0440 (13)	0.093 (2)	−0.0129 (11)	−0.0158 (13)	0.0033 (13)
C5	0.0456 (13)	0.0493 (13)	0.0637 (15)	−0.0210 (11)	−0.0105 (11)	−0.0018 (11)
C6	0.0384 (16)	0.082 (3)	0.202 (6)	−0.0174 (17)	0.005 (2)	0.052 (3)
C7	0.138 (5)	0.176 (6)	0.143 (5)	−0.121 (5)	0.084 (4)	−0.089 (4)
C8	0.116 (3)	0.182 (5)	0.082 (3)	−0.103 (4)	−0.036 (2)	0.053 (3)
C9	0.074 (2)	0.081 (2)	0.127 (3)	−0.0502 (19)	−0.029 (2)	0.037 (2)
C10	0.067 (2)	0.133 (4)	0.110 (3)	−0.067 (2)	−0.034 (2)	0.036 (3)
C11	0.0382 (11)	0.0468 (12)	0.0458 (12)	−0.0232 (9)	−0.0104 (9)	0.0030 (9)
C12	0.0429 (12)	0.0456 (12)	0.0517 (13)	−0.0192 (10)	−0.0159 (10)	0.0001 (10)
C13	0.0518 (13)	0.0409 (12)	0.0584 (14)	−0.0187 (10)	−0.0163 (11)	0.0043 (10)
C14	0.0454 (12)	0.0420 (12)	0.0518 (13)	−0.0117 (10)	−0.0190 (11)	0.0020 (10)
C15	0.0695 (18)	0.0727 (18)	0.0577 (16)	−0.0324 (14)	−0.0173 (13)	−0.0090 (13)
C16	0.110 (3)	0.098 (3)	0.0526 (17)	−0.040 (2)	−0.0206 (18)	−0.0092 (16)
C17	0.094 (3)	0.092 (2)	0.0623 (19)	−0.033 (2)	−0.0009 (18)	0.0047 (17)
C18	0.070 (2)	0.084 (2)	0.082 (2)	−0.0381 (17)	−0.0089 (17)	0.0137 (17)
C19	0.0534 (14)	0.0577 (15)	0.0657 (16)	−0.0227 (12)	−0.0196 (12)	0.0005 (12)
C20	0.172 (6)	0.180 (6)	0.074 (3)	−0.069 (5)	0.028 (3)	−0.001 (3)

Geometric parameters (Å, º)

Fe1—C7	2.019 (4)	C7—C8	1.436 (8)
Fe1—C8	2.020 (4)	C7—H7	0.9300
Fe1—C6	2.025 (3)	C8—C9	1.339 (6)
Fe1—C1	2.026 (2)	C8—H8	0.9300
Fe1—C9	2.036 (3)	C9—C10	1.347 (5)
Fe1—C5	2.037 (3)	C9—H9	0.9300
Fe1—C2	2.040 (2)	C10—H10	0.9300
Fe1—C10	2.046 (3)	C11—C12	1.512 (3)
Fe1—C4	2.059 (3)	C12—C13	1.524 (3)
Fe1—C3	2.061 (3)	C12—H12B	0.9700
O1—C11	1.225 (3)	C12—H12A	0.9700
N1—C14	1.386 (3)	C13—H13B	0.9700

N1—C13	1.458 (3)	C13—H13A	0.9700
N1—H1N	0.82 (3)	C14—C15	1.400 (4)
C1—C2	1.433 (3)	C14—C19	1.401 (4)
C1—C5	1.433 (3)	C15—C16	1.380 (5)
C1—C11	1.466 (3)	C15—H15	0.9300
C2—C3	1.413 (4)	C16—C17	1.379 (6)
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.410 (4)	C17—C18	1.400 (5)
C3—H3	0.9300	C17—C20	1.520 (5)
C4—C5	1.416 (4)	C18—C19	1.370 (4)
C4—H4	0.9300	C18—H18	0.9300
C5—H5	0.9300	C19—H19	0.9300
C6—C10	1.351 (7)	C20—H20A	0.9600
C6—C7	1.417 (8)	C20—H20B	0.9600
C6—H6	0.9300	C20—H20C	0.9600

C7—Fe1—C8	41.7 (2)	C1—C5—Fe1	68.92 (14)
C7—Fe1—C6	41.0 (2)	C4—C5—H5	126.0
C8—Fe1—C6	67.5 (2)	C1—C5—H5	126.0
C7—Fe1—C1	122.9 (2)	Fe1—C5—H5	126.1
C8—Fe1—C1	160.1 (2)	C10—C6—C7	108.9 (4)
C6—Fe1—C1	109.62 (13)	C10—C6—Fe1	71.4 (2)
C7—Fe1—C9	67.37 (19)	C7—C6—Fe1	69.3 (2)
C8—Fe1—C9	38.55 (19)	C10—C6—H6	125.5
C6—Fe1—C9	65.48 (16)	C7—C6—H6	125.5
C1—Fe1—C9	159.90 (15)	Fe1—C6—H6	125.3
C7—Fe1—C5	158.2 (3)	C6—C7—C8	103.8 (4)
C8—Fe1—C5	157.6 (2)	C6—C7—Fe1	69.7 (2)
C6—Fe1—C5	121.7 (2)	C8—C7—Fe1	69.2 (2)
C1—Fe1—C5	41.30 (10)	C6—C7—H7	128.1
C9—Fe1—C5	122.86 (15)	C8—C7—H7	128.1
C7—Fe1—C2	109.55 (16)	Fe1—C7—H7	124.7
C8—Fe1—C2	123.88 (17)	C9—C8—C7	108.2 (4)
C6—Fe1—C2	128.16 (18)	C9—C8—Fe1	71.4 (2)
C1—Fe1—C2	41.26 (10)	C7—C8—Fe1	69.2 (2)
C9—Fe1—C2	157.13 (14)	C9—C8—H8	125.9
C5—Fe1—C2	68.80 (11)	C7—C8—H8	125.9
C7—Fe1—C10	67.3 (2)	Fe1—C8—H8	125.1
C8—Fe1—C10	65.57 (17)	C8—C9—C10	110.1 (4)
C6—Fe1—C10	38.8 (2)	C8—C9—Fe1	70.1 (2)
C1—Fe1—C10	125.38 (13)	C10—C9—Fe1	71.1 (2)
C9—Fe1—C10	38.54 (15)	C8—C9—H9	125.0
C5—Fe1—C10	107.63 (15)	C10—C9—H9	125.0
C2—Fe1—C10	163.31 (14)	Fe1—C9—H9	125.4
C7—Fe1—C4	160.8 (3)	C9—C10—C6	109.0 (5)
C8—Fe1—C4	122.6 (2)	C9—C10—Fe1	70.33 (19)
C6—Fe1—C4	155.2 (2)	C6—C10—Fe1	69.8 (2)
C1—Fe1—C4	68.69 (10)	C9—C10—H10	125.5

C9—Fe1—C4	107.10 (14)	C6—C10—H10	125.5
C5—Fe1—C4	40.44 (11)	Fe1—C10—H10	125.9
C2—Fe1—C4	67.92 (11)	O1—C11—C1	121.2 (2)
C10—Fe1—C4	120.67 (17)	O1—C11—C12	120.6 (2)
C7—Fe1—C3	125.8 (3)	C1—C11—C12	118.20 (19)
C8—Fe1—C3	108.53 (16)	C11—C12—C13	112.77 (19)
C6—Fe1—C3	164.3 (2)	C11—C12—H12B	109.0
C1—Fe1—C3	68.62 (10)	C13—C12—H12B	109.0
C9—Fe1—C3	121.62 (14)	C11—C12—H12A	109.0
C5—Fe1—C3	67.99 (12)	C13—C12—H12A	109.0
C2—Fe1—C3	40.30 (11)	H12B—C12—H12A	107.8
C10—Fe1—C3	155.02 (16)	N1—C13—C12	113.48 (19)
C4—Fe1—C3	40.02 (12)	N1—C13—H13B	108.9
C14—N1—C13	121.9 (2)	C12—C13—H13B	108.9
C14—N1—H1N	116.2 (19)	N1—C13—H13A	108.9
C13—N1—H1N	109.9 (19)	C12—C13—H13A	108.9
C2—C1—C5	107.0 (2)	H13B—C13—H13A	107.7
C2—C1—C11	127.8 (2)	N1—C14—C15	123.3 (2)
C5—C1—C11	125.0 (2)	N1—C14—C19	119.4 (2)
C2—C1—Fe1	69.89 (13)	C15—C14—C19	117.2 (2)
C5—C1—Fe1	69.78 (14)	C16—C15—C14	120.3 (3)
C11—C1—Fe1	121.59 (15)	C16—C15—H15	119.9
C3—C2—C1	108.1 (2)	C14—C15—H15	119.9
C3—C2—Fe1	70.65 (14)	C17—C16—C15	123.0 (3)
C1—C2—Fe1	68.85 (13)	C17—C16—H16	118.5
C3—C2—H2	125.9	C15—C16—H16	118.5
C1—C2—H2	125.9	C16—C17—C18	116.4 (3)
Fe1—C2—H2	126.1	C16—C17—C20	122.3 (4)
C4—C3—C2	108.5 (2)	C18—C17—C20	121.3 (4)
C4—C3—Fe1	69.92 (15)	C19—C18—C17	121.9 (3)
C2—C3—Fe1	69.06 (14)	C19—C18—H18	119.1
C4—C3—H3	125.8	C17—C18—H18	119.1
C2—C3—H3	125.8	C18—C19—C14	121.3 (3)
Fe1—C3—H3	126.8	C18—C19—H19	119.4
C3—C4—C5	108.4 (2)	C14—C19—H19	119.4
C3—C4—Fe1	70.06 (16)	C17—C20—H20A	109.5
C5—C4—Fe1	68.96 (15)	C17—C20—H20B	109.5
C3—C4—H4	125.8	H20A—C20—H20B	109.5
C5—C4—H4	125.8	C17—C20—H20C	109.5
Fe1—C4—H4	126.7	H20A—C20—H20C	109.5
C4—C5—C1	108.0 (2)	H20B—C20—H20C	109.5
C4—C5—Fe1	70.60 (17)		

C7—Fe1—C1—C2	82.4 (3)	C2—Fe1—C6—C10	165.2 (2)
C8—Fe1—C1—C2	48.2 (5)	C4—Fe1—C6—C10	41.1 (5)
C6—Fe1—C1—C2	126.0 (3)	C3—Fe1—C6—C10	−156.8 (4)
C9—Fe1—C1—C2	−161.9 (4)	C8—Fe1—C6—C7	41.0 (3)
C5—Fe1—C1—C2	−117.8 (2)	C1—Fe1—C6—C7	−118.0 (3)

C10—Fe1—C1—C2	166.4 (2)	C9—Fe1—C6—C7	83.1 (3)
C4—Fe1—C1—C2	−80.38 (17)	C5—Fe1—C6—C7	−162.1 (3)
C3—Fe1—C1—C2	−37.27 (16)	C2—Fe1—C6—C7	−75.2 (3)
C7—Fe1—C1—C5	−159.8 (3)	C10—Fe1—C6—C7	119.5 (4)
C8—Fe1—C1—C5	166.0 (5)	C4—Fe1—C6—C7	160.6 (4)
C6—Fe1—C1—C5	−116.1 (3)	C3—Fe1—C6—C7	−37.3 (6)
C9—Fe1—C1—C5	−44.1 (4)	C10—C6—C7—C8	−0.5 (4)
C2—Fe1—C1—C5	117.8 (2)	Fe1—C6—C7—C8	−61.2 (3)
C10—Fe1—C1—C5	−75.8 (2)	C10—C6—C7—Fe1	60.7 (3)
C4—Fe1—C1—C5	37.45 (16)	C8—Fe1—C7—C6	−114.4 (4)
C3—Fe1—C1—C5	80.56 (17)	C1—Fe1—C7—C6	82.3 (3)
C7—Fe1—C1—C11	−40.4 (4)	C9—Fe1—C7—C6	−78.1 (3)
C8—Fe1—C1—C11	−74.6 (5)	C5—Fe1—C7—C6	44.6 (5)
C6—Fe1—C1—C11	3.2 (3)	C2—Fe1—C7—C6	126.2 (3)
C9—Fe1—C1—C11	75.3 (4)	C10—Fe1—C7—C6	−36.2 (3)
C5—Fe1—C1—C11	119.4 (2)	C4—Fe1—C7—C6	−154.9 (4)
C2—Fe1—C1—C11	−122.8 (2)	C3—Fe1—C7—C6	168.3 (2)
C10—Fe1—C1—C11	43.6 (3)	C6—Fe1—C7—C8	114.4 (4)
C4—Fe1—C1—C11	156.8 (2)	C1—Fe1—C7—C8	−163.3 (2)
C3—Fe1—C1—C11	−160.1 (2)	C9—Fe1—C7—C8	36.3 (3)
C5—C1—C2—C3	−0.2 (3)	C5—Fe1—C7—C8	159.0 (3)
C11—C1—C2—C3	174.9 (2)	C2—Fe1—C7—C8	−119.4 (3)
Fe1—C1—C2—C3	59.96 (18)	C10—Fe1—C7—C8	78.2 (3)
C5—C1—C2—Fe1	−60.20 (16)	C4—Fe1—C7—C8	−40.5 (6)
C11—C1—C2—Fe1	115.0 (2)	C3—Fe1—C7—C8	−77.3 (3)
C7—Fe1—C2—C3	122.7 (4)	C6—C7—C8—C9	0.6 (4)
C8—Fe1—C2—C3	78.5 (3)	Fe1—C7—C8—C9	−61.0 (3)
C6—Fe1—C2—C3	165.0 (3)	C6—C7—C8—Fe1	61.6 (3)
C1—Fe1—C2—C3	−119.3 (2)	C7—Fe1—C8—C9	118.8 (4)
C9—Fe1—C2—C3	44.8 (4)	C6—Fe1—C8—C9	78.4 (3)
C5—Fe1—C2—C3	−80.56 (19)	C1—Fe1—C8—C9	163.9 (3)
C10—Fe1—C2—C3	−161.2 (5)	C5—Fe1—C8—C9	−40.7 (5)
C4—Fe1—C2—C3	−36.92 (18)	C2—Fe1—C8—C9	−159.8 (2)
C7—Fe1—C2—C1	−118.0 (3)	C10—Fe1—C8—C9	36.1 (3)
C8—Fe1—C2—C1	−162.2 (2)	C4—Fe1—C8—C9	−75.9 (3)
C6—Fe1—C2—C1	−75.6 (3)	C3—Fe1—C8—C9	−117.8 (3)
C9—Fe1—C2—C1	164.1 (4)	C6—Fe1—C8—C7	−40.3 (3)
C5—Fe1—C2—C1	38.75 (14)	C1—Fe1—C8—C7	45.2 (6)
C10—Fe1—C2—C1	−41.9 (5)	C9—Fe1—C8—C7	−118.8 (4)
C4—Fe1—C2—C1	82.40 (16)	C5—Fe1—C8—C7	−159.5 (4)
C3—Fe1—C2—C1	119.3 (2)	C2—Fe1—C8—C7	81.5 (4)
C1—C2—C3—C4	0.1 (3)	C10—Fe1—C8—C7	−82.7 (4)
Fe1—C2—C3—C4	58.98 (19)	C4—Fe1—C8—C7	165.3 (3)
C1—C2—C3—Fe1	−58.84 (17)	C3—Fe1—C8—C7	123.4 (3)
C7—Fe1—C3—C4	162.2 (3)	C7—C8—C9—C10	−0.5 (4)
C8—Fe1—C3—C4	119.0 (3)	Fe1—C8—C9—C10	−60.1 (3)
C6—Fe1—C3—C4	−168.5 (5)	C7—C8—C9—Fe1	59.6 (3)
C1—Fe1—C3—C4	−81.91 (17)	C7—Fe1—C9—C8	−39.1 (4)

C9—Fe1—C3—C4	78.7 (2)	C6—Fe1—C9—C8	−84.1 (4)
C5—Fe1—C3—C4	−37.31 (16)	C1—Fe1—C9—C8	−164.1 (4)
C2—Fe1—C3—C4	−120.1 (2)	C5—Fe1—C9—C8	162.7 (3)
C10—Fe1—C3—C4	47.3 (4)	C2—Fe1—C9—C8	47.7 (5)
C7—Fe1—C3—C2	−77.8 (3)	C10—Fe1—C9—C8	−120.7 (4)
C8—Fe1—C3—C2	−120.9 (3)	C4—Fe1—C9—C8	121.3 (3)
C6—Fe1—C3—C2	−48.4 (6)	C3—Fe1—C9—C8	80.0 (3)
C1—Fe1—C3—C2	38.14 (16)	C7—Fe1—C9—C10	81.5 (4)
C9—Fe1—C3—C2	−161.3 (2)	C8—Fe1—C9—C10	120.7 (4)
C5—Fe1—C3—C2	82.74 (18)	C6—Fe1—C9—C10	36.6 (3)
C10—Fe1—C3—C2	167.4 (3)	C1—Fe1—C9—C10	−43.4 (5)
C4—Fe1—C3—C2	120.1 (2)	C5—Fe1—C9—C10	−76.6 (3)
C2—C3—C4—C5	0.0 (3)	C2—Fe1—C9—C10	168.3 (3)
Fe1—C3—C4—C5	58.46 (18)	C4—Fe1—C9—C10	−118.0 (3)
C2—C3—C4—Fe1	−58.45 (19)	C3—Fe1—C9—C10	−159.3 (3)
C7—Fe1—C4—C3	−49.0 (5)	C8—C9—C10—C6	0.1 (4)
C8—Fe1—C4—C3	−79.9 (2)	Fe1—C9—C10—C6	−59.3 (2)
C6—Fe1—C4—C3	172.6 (3)	C8—C9—C10—Fe1	59.4 (3)
C1—Fe1—C4—C3	81.73 (16)	C7—C6—C10—C9	0.3 (4)
C9—Fe1—C4—C3	−119.1 (2)	Fe1—C6—C10—C9	59.6 (3)
C5—Fe1—C4—C3	119.9 (2)	C7—C6—C10—Fe1	−59.3 (3)
C2—Fe1—C4—C3	37.16 (16)	C7—Fe1—C10—C9	−81.7 (4)
C10—Fe1—C4—C3	−158.85 (19)	C8—Fe1—C10—C9	−36.1 (3)
C7—Fe1—C4—C5	−169.0 (4)	C6—Fe1—C10—C9	−119.9 (4)
C8—Fe1—C4—C5	160.2 (2)	C1—Fe1—C10—C9	163.2 (2)
C6—Fe1—C4—C5	52.6 (4)	C5—Fe1—C10—C9	121.0 (3)
C1—Fe1—C4—C5	−38.22 (15)	C2—Fe1—C10—C9	−164.1 (4)
C9—Fe1—C4—C5	120.94 (19)	C4—Fe1—C10—C9	78.7 (3)
C2—Fe1—C4—C5	−82.78 (16)	C3—Fe1—C10—C9	45.4 (5)
C10—Fe1—C4—C5	81.2 (2)	C7—Fe1—C10—C6	38.3 (3)
C3—Fe1—C4—C5	−119.9 (2)	C8—Fe1—C10—C6	83.9 (4)
C3—C4—C5—C1	−0.2 (3)	C1—Fe1—C10—C6	−76.9 (3)
Fe1—C4—C5—C1	58.98 (17)	C9—Fe1—C10—C6	119.9 (4)
C3—C4—C5—Fe1	−59.1 (2)	C5—Fe1—C10—C6	−119.1 (3)
C2—C1—C5—C4	0.2 (3)	C2—Fe1—C10—C6	−44.2 (6)
C11—C1—C5—C4	−175.1 (2)	C4—Fe1—C10—C6	−161.3 (3)
Fe1—C1—C5—C4	−60.03 (18)	C3—Fe1—C10—C6	165.3 (4)
C2—C1—C5—Fe1	60.27 (16)	C2—C1—C11—O1	179.4 (2)
C11—C1—C5—Fe1	−115.1 (2)	C5—C1—C11—O1	−6.2 (3)
C7—Fe1—C5—C4	170.3 (4)	Fe1—C1—C11—O1	−92.5 (2)
C8—Fe1—C5—C4	−48.4 (4)	C2—C1—C11—C12	1.5 (3)
C6—Fe1—C5—C4	−156.9 (2)	C5—C1—C11—C12	175.9 (2)
C1—Fe1—C5—C4	119.1 (2)	Fe1—C1—C11—C12	89.6 (2)
C9—Fe1—C5—C4	−77.4 (2)	O1—C11—C12—C13	12.3 (3)
C2—Fe1—C5—C4	80.42 (17)	C1—C11—C12—C13	−169.82 (19)
C10—Fe1—C5—C4	−116.9 (2)	C14—N1—C13—C12	69.9 (3)
C3—Fe1—C5—C4	36.94 (16)	C11—C12—C13—N1	70.6 (3)
C7—Fe1—C5—C1	51.1 (5)	C13—N1—C14—C15	21.2 (4)

C8—Fe1—C5—C1	−167.6 (4)	C13—N1—C14—C19	−162.0 (2)
C6—Fe1—C5—C1	83.9 (2)	N1—C14—C15—C16	176.1 (3)
C9—Fe1—C5—C1	163.46 (17)	C19—C14—C15—C16	−0.8 (4)
C2—Fe1—C5—C1	−38.73 (14)	C14—C15—C16—C17	0.0 (6)
C10—Fe1—C5—C1	123.97 (19)	C15—C16—C17—C18	0.6 (6)
C4—Fe1—C5—C1	−119.1 (2)	C15—C16—C17—C20	−179.8 (4)
C3—Fe1—C5—C1	−82.20 (16)	C16—C17—C18—C19	−0.6 (6)
C7—Fe1—C6—C10	−119.5 (4)	C20—C17—C18—C19	179.8 (4)
C8—Fe1—C6—C10	−78.6 (3)	C17—C18—C19—C14	−0.2 (5)
C1—Fe1—C6—C10	122.5 (3)	N1—C14—C19—C18	−176.1 (3)
C9—Fe1—C6—C10	−36.4 (3)	C15—C14—C19—C18	0.9 (4)
C5—Fe1—C6—C10	78.4 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1^{i}	0.82 (3)	2.31 (4)	3.102 (4)	161 (3)
C19—H19···O1^{i}	0.93	2.69	3.455 (4)	140
C4—H4···N1^{ii}	0.93	2.64	3.451 (4)	147

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*+1, *y*−1, *z*.