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ISSN 2414-3146

N-Ferrocenymethyl-*N*-phenylacetamide

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Received 18 January 2016
Accepted 2 February 2016

Edited by J. Simpson, University of Otago, New Zealand

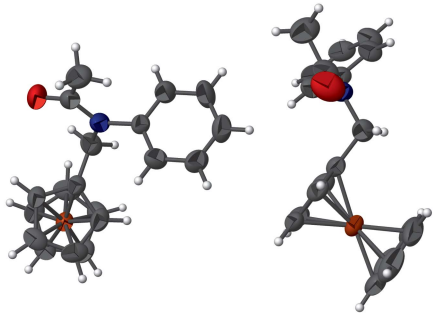
Keywords: crystal structure; *N*-ferrocenymethyl-*N*-phenylacetamide; hydrogen bonding.

CCDC reference: 1451430

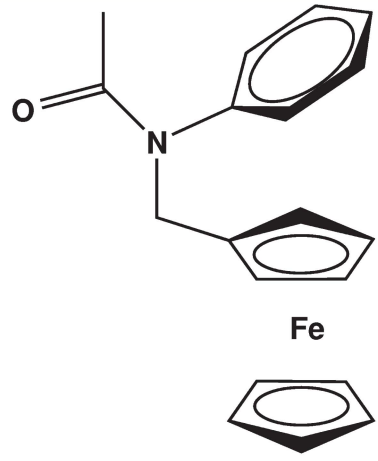
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Fe(C_5H_5)(C_{14}H_{14}NO)]$, the asymmetric unit comprises two unique molecules. The two cyclopentadienyl (Cp) rings of each ferrocene residue are nearly parallel to one another. In each substituted Cp ring, the CH_2 group carries an *N*-phenylacetamide residue. In the crystal, C—H···O hydrogen bonds stack molecules along *a*.

3D view



Chemical scheme



Structure description

Ferrocene and its derivatives are known to be of considerable interest, because of their use in organic synthesis (Khand *et al.*, 1989), catalysis (Szarka *et al.*, 2004), materials science (Uno & Dixneuf, 1998), asymmetric synthesis (Torres *et al.*, 2002), medicinal chemistry (Chavain *et al.*, 2009) and electrochemistry (Ahmedi & Lanez, 2011; Khelef & Lanez, 2015). As a continuation of our research related to ferrocene derivatives (Khelef *et al.*, 2012; Rahim *et al.*, 2012), we report the synthesis and structural characterization of the title compound.

The asymmetric unit of title compound comprises two crystallographically independent molecules, *A* and *B* (Fig. 1). The two cyclopentadienyl (Cp) rings of each ferrocene residue are nearly parallel to one another, the dihedral angle between the mean planes of Cp1/Cp2 is 3.2 (2)° and Cp3/Cp4 is 2.6 (2)° (Cp1 = C1*A*–C5*A*, Cp2 = C6*A*–C10*A*, Cp2 = C1*B*–C5*B* and Cp4 = C6*B*–C10*B*). The Cp rings are essentially parallel and the Fe···centroid distances are 1.648 (3) (Cp1), 1.640 (3) (Cp2), 1.652 (3) (Cp3) and 1.645 (3) Å (Cp4). The [*Cg*1···Fe1···*Cg*2] angle is 178.16 (2)° and [*Cg*3···Fe2···*Cg*4] angle is 179.21 (2)° [*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the Cp1, Cp2, Cp3 and Cp4 rings, respectively].

In each molecule one of the Cp rings is substituted by an amide group which is essentially perpendicular to the substituted cyclopentadienyl ring [torsion angles C14*A*—N1—C11*A*—C10*A* and C14*B*—N2—C11*B*—C10*B* are 93.3 (4) and −93.3 (4)°, respec-

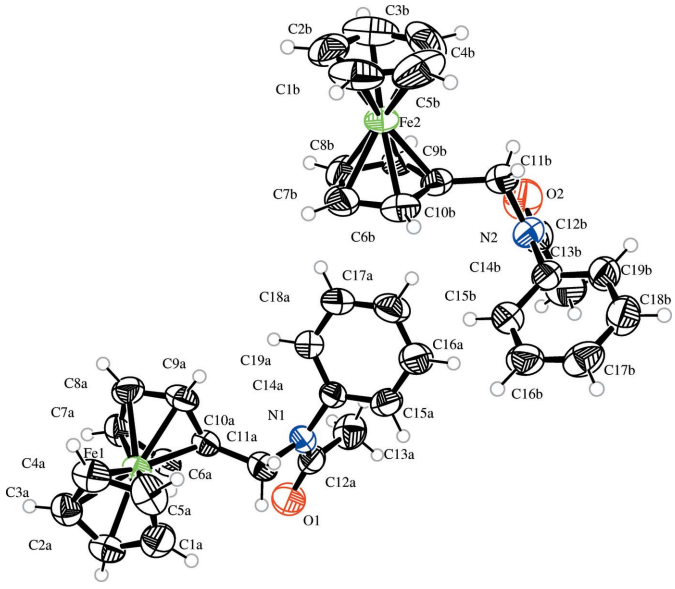


Figure 1
The molecular structure of the title compound, showing the atomic numbering scheme and 50% probability displacement ellipsoids.

tively]. In the methanoyl group, the N and O atoms are coplanar [the C11*A*—N1—C12*A*—O1 torsion angle is −0.6 (5)° and the C11*B*—N2—C12*B*—O2 torsion angle is −2.9 (6)°]. In the crystal, C—H···O hydrogen bonds, Table 1, combine to stack the molecules along the *a* axis, Fig. 2.

Synthesis and crystallization

N-ferrocenylmethylaniline was obtained as described in the literature (Osgerby & Pauson, 1961). To a 250 ml round-bottom flask equipped with a reflux condenser and a magnetic stirrer a suspension of *N*-ferrocenylmethylaniline (6 g, 20 mmol) in 50 ml of dry toluene was added under a nitrogen atmosphere. The resulting suspension was heated at 50°C until all the solid materials had dissolved completely. 50 ml of anhydride acetic acid was then added and the resulting mixture was vigorously stirred under reflux for 20 min. The reaction mixture was then poured into water; the organic layer was separated, washed twice with water, dried over $MgSO_4$ and evaporated. The residue was recrystallized from a mixture of ethanol–water to yield *N*-ferrocenymethyl-*N*-phenyl-acetamide as orange needles (yield: 5.6 g, 81.5%; m.p. 116–117°C). The compounds gave clean ^{1}H and ^{13}C NMR spectra in $CDCl_3$. NMR ^{1}H (300 MHz, $CDCl_3$) 1.75 (*s*, 3H, CH_3), 4.03 (*s*, 4H, C_5H_4), 4.08 (*s*, 5H, C_5H_5), 4.61 (*s*, 2H, CH_2), 6.99 (*d*, 2H, *ortho*-C_6H_5), 7.28–7.35 (*m*, 3H, *meta*- and *para*-C_6H_5). NMR ^{13}C (75 MHz, $CDCl_3$) 22.83 (1C, CH_3), 48.40 (1C, CH_2), 68.13, 69.89 and 83.13 (5C, C5H4), 68.55 (5C, C_5H_5), 127.87, 128.55, 129.43, 142.84 (6C, C_6H_5), 169.74 (1C, CO).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15*A*—H15*A*···O1^{i}	0.93	2.56	3.456 (5)	162
C19*B*—H19*B*···O2^{ii}	0.93	2.55	3.421 (5)	157
C15*A*—H15*A*···O1^{i}	0.93	2.56	3.456 (5)	162
C19*B*—H19*B*···O2^{ii}	0.93	2.55	3.421 (5)	157

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

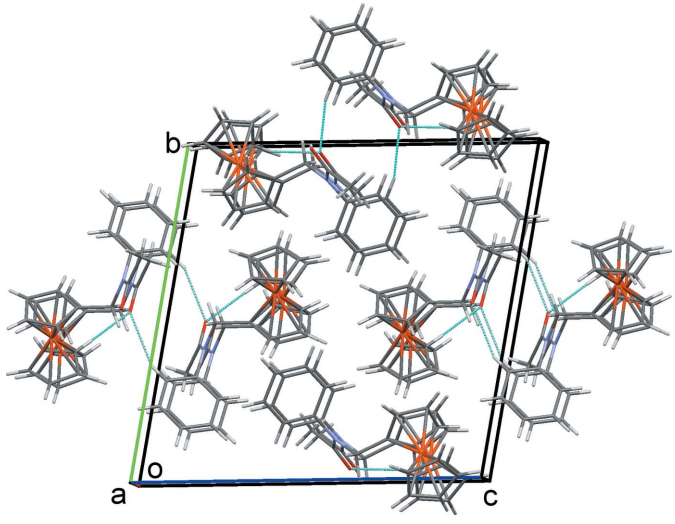


Figure 2
The crystal packing of the title compound, viewed along the *b* axis, with hydrogen bonds drawn as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_5H_5)(C_{14}H_{14}NO)]$
M_r	333.2
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	298
a, *b*, *c* (Å)	7.344 (1), 14.831 (1), 15.267 (1)
α, β, γ (°)	79.094 (10), 79.627 (10), 87.508 (10)
V (Å^3)	1606.1 (3)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.94
Crystal size (mm)	0.3 × 0.1 × 0.1
Data collection	
Diffractometer	Nonius KappaCCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8635, 5157, 3765
R_{int}	0.039
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.588
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.042, 0.115, 1.02
No. of reflections	5157
No. of parameters	398
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.28

Computer programs: *COLLECT* (Nonius, 1998), *SIR92* (Altomare *et al.*, 1993), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *WinGX* (Farrugia, 2012).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

This research was financed by the Laboratory of Valorization and Promotion of Saharan resources (project No. E03220080002). The authors acknowledge the assistance of Merazig Hocine for the data collection.

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full crystallographic data

IUCrData (2016). **1**, x160203 [https://doi.org/10.1107/S2414314616002030]

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N-Ferrocenymethyl-*N*-phenylacetamide

Crystal data

$[Fe(C_5H_5)(C_{14}H_{14}NO)]$
M_r = 333.2
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.344 (1) Å
b = 14.831 (1) Å
c = 15.267 (1) Å
α = 79.094 (10)°
β = 79.627 (10)°
γ = 87.508 (10)°
V = 1606.1 (3) Å^3
Z = 4
$F(000)$ = 696
D_x = 1.378 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5157 reflections
θ = 2.8–24.7°
μ = 0.94 mm^{-1}
T = 298 K
Needle, orange
0.3 × 0.1 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
CCD scans
8635 measured reflections
5157 independent reflections
3765 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 24.7°, θ_{min} = 2.8°
h = −8→8
k = −17→17
l = −15→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.115
S = 1.02
5157 reflections
398 parameters
0 restraints
0 constraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.6059P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0049 (12)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe2	0.46219 (6)	0.43859 (3)	0.69245 (3)	0.04595 (17)
Fe1	0.06009 (6)	0.92687 (3)	0.17945 (3)	0.04206 (17)
O1	−0.5391 (4)	0.9627 (2)	0.3939 (2)	0.0854 (10)
C14A	−0.2433 (5)	0.8074 (2)	0.5143 (2)	0.0462 (8)
N2	0.1143 (4)	0.6002 (2)	0.8775 (2)	0.0570 (8)
C10B	0.2785 (5)	0.5231 (2)	0.7548 (2)	0.0473 (8)
N1	−0.3111 (4)	0.8744 (2)	0.44649 (18)	0.0524 (7)
O2	−0.1384 (5)	0.5145 (2)	0.8928 (2)	0.0918 (10)
C3A	0.2181 (5)	0.9949 (3)	0.0637 (3)	0.0555 (9)
H3A	0.2196	0.9852	0.0051	0.067*
C10A	−0.1303 (4)	0.8808 (2)	0.2910 (2)	0.0445 (8)
C7A	−0.1331 (5)	0.8472 (3)	0.1509 (3)	0.0578 (10)
H7A	−0.1637	0.8476	0.0943	0.069*
C1B	0.7309 (6)	0.4029 (3)	0.6688 (5)	0.0860 (16)
H1B	0.8239	0.4413	0.6337	0.103*
C14B	0.2045 (5)	0.6821 (2)	0.8845 (2)	0.0510 (9)
C11A	−0.1712 (6)	0.9246 (3)	0.3737 (2)	0.0610 (10)
H11A	−0.0575	0.9277	0.3969	0.073*
H11B	−0.215	0.987	0.3565	0.073*
C5A	0.2862 (6)	0.9844 (3)	0.2041 (3)	0.0702 (12)
H5A	0.3401	0.9666	0.2554	0.084*
C9B	0.1873 (5)	0.4692 (3)	0.7081 (3)	0.0560 (10)
H10B	0.0918	0.4282	0.7341	0.067*
C6B	0.4137 (5)	0.5750 (2)	0.6887 (3)	0.0600 (10)
H8B	0.4938	0.6167	0.7	0.072*
C8B	0.2676 (6)	0.4892 (3)	0.6154 (3)	0.0670 (12)
H6B	0.2336	0.4638	0.5695	0.08*
C15B	0.2566 (6)	0.7485 (3)	0.8087 (3)	0.0630 (10)
H15B	0.2272	0.7424	0.7534	0.076*
C19A	−0.1770 (6)	0.7239 (3)	0.4957 (3)	0.0623 (10)
H19A	−0.1825	0.7092	0.4397	0.075*
C16A	−0.1674 (7)	0.7642 (3)	0.6620 (3)	0.0860 (15)
H16A	−0.1669	0.7775	0.7191	0.103*
C15A	−0.2392 (6)	0.8279 (3)	0.5980 (3)	0.0701 (12)
H15A	−0.2843	0.8842	0.6116	0.084*
C11B	0.2372 (6)	0.5234 (3)	0.8542 (3)	0.0638 (10)
H11C	0.1794	0.4658	0.8854	0.077*
H11D	0.3526	0.5274	0.8757	0.077*
C19B	0.2455 (5)	0.6916 (3)	0.9662 (3)	0.0593 (10)
H19B	0.2109	0.6467	1.0174	0.071*
C16B	0.3528 (6)	0.8243 (3)	0.8152 (3)	0.0693 (12)
H16B	0.3899	0.8686	0.7639	0.083*
C7B	0.4077 (6)	0.5539 (3)	0.6044 (3)	0.0683 (12)
H7B	0.4833	0.5783	0.5502	0.082*
C17B	0.3936 (5)	0.8344 (3)	0.8966 (3)	0.0687 (11)

H17B	0.458	0.8855	0.901	0.082*
C13B	−0.1921 (6)	0.6659 (3)	0.9251 (3)	0.0840 (14)
H13D	−0.1149	0.7167	0.9247	0.126*
H13E	−0.2758	0.6843	0.8833	0.126*
H13F	−0.2614	0.6468	0.985	0.126*
C18B	0.3386 (6)	0.7683 (3)	0.9719 (3)	0.0715 (12)
H18B	0.3646	0.7755	1.0276	0.086*
C18A	−0.1024 (6)	0.6619 (3)	0.5591 (3)	0.0678 (11)
H18A	−0.0554	0.606	0.5452	0.081*
C12B	−0.0721 (6)	0.5868 (3)	0.8974 (3)	0.0661 (11)
C13A	−0.6325 (5)	0.8459 (3)	0.5234 (3)	0.0755 (12)
H13A	−0.5703	0.7993	0.5603	0.113*
H13B	−0.6982	0.8867	0.5602	0.113*
H13C	−0.7184	0.8176	0.4966	0.113*
C5B	0.6691 (9)	0.3963 (4)	0.7606 (5)	0.108 (2)
H5B	0.7128	0.4286	0.7991	0.13*
C12A	−0.4920 (6)	0.8994 (3)	0.4496 (3)	0.0603 (10)
C3B	0.5097 (7)	0.3011 (3)	0.7083 (5)	0.0904 (17)
H3B	0.4254	0.2576	0.7046	0.108*
C17A	−0.0971 (6)	0.6820 (3)	0.6423 (3)	0.0712 (12)
H17A	−0.0463	0.6403	0.6851	0.085*
C2B	0.6325 (7)	0.3434 (4)	0.6386 (4)	0.0820 (14)
H2B	0.6478	0.3336	0.5793	0.098*
C4B	0.5260 (8)	0.3308 (5)	0.7846 (4)	0.104 (2)
H4B	0.4566	0.3118	0.842	0.125*
C6A	−0.2156 (4)	0.9027 (2)	0.2139 (2)	0.0473 (8)
H6A	−0.3095	0.946	0.2058	0.057*
C9A	0.0048 (5)	0.8118 (2)	0.2743 (3)	0.0565 (10)
H9A	0.0823	0.7844	0.3139	0.068*
C2A	0.1019 (5)	1.0569 (3)	0.1067 (3)	0.0598 (10)
H2A	0.0129	1.0951	0.0821	0.072*
C8A	0.0022 (6)	0.7917 (3)	0.1888 (3)	0.0643 (11)
H8A	0.0774	0.7489	0.1617	0.077*
C4A	0.3312 (5)	0.9501 (3)	0.1231 (3)	0.0606 (10)
H4A	0.4205	0.9056	0.1111	0.073*
C1A	0.1441 (6)	1.0510 (3)	0.1936 (3)	0.0699 (12)
H1A	0.0884	1.0849	0.2368	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe2	0.0372 (3)	0.0402 (3)	0.0616 (3)	0.0043 (2)	−0.0144 (2)	−0.0080 (2)
Fe1	0.0369 (3)	0.0396 (3)	0.0473 (3)	−0.00241 (19)	−0.0069 (2)	−0.0021 (2)
O1	0.109 (2)	0.079 (2)	0.0712 (19)	0.0397 (18)	−0.0356 (17)	−0.0112 (17)
C14A	0.0495 (19)	0.043 (2)	0.0428 (19)	0.0045 (15)	−0.0064 (14)	−0.0025 (16)
N2	0.071 (2)	0.0462 (18)	0.0552 (19)	0.0011 (15)	−0.0074 (15)	−0.0164 (15)
C10B	0.047 (2)	0.041 (2)	0.058 (2)	0.0054 (15)	−0.0164 (16)	−0.0133 (17)
N1	0.0625 (19)	0.0486 (18)	0.0406 (16)	0.0073 (14)	−0.0026 (13)	−0.0021 (14)

O2	0.107 (3)	0.076 (2)	0.091 (2)	−0.0400 (19)	−0.0019 (18)	−0.0184 (18)
C3A	0.053 (2)	0.058 (2)	0.055 (2)	−0.0172 (18)	−0.0041 (17)	−0.0073 (19)
C10A	0.0441 (19)	0.0402 (19)	0.0457 (19)	−0.0021 (14)	−0.0062 (14)	−0.0005 (15)
C7A	0.063 (2)	0.058 (2)	0.049 (2)	−0.0259 (19)	−0.0017 (17)	−0.0067 (19)
C1B	0.049 (3)	0.053 (3)	0.140 (5)	0.005 (2)	−0.009 (3)	0.014 (3)
C14B	0.056 (2)	0.045 (2)	0.051 (2)	0.0004 (16)	−0.0041 (16)	−0.0131 (17)
C11A	0.077 (3)	0.051 (2)	0.051 (2)	−0.0078 (19)	−0.0100 (19)	−0.0004 (18)
C5A	0.059 (3)	0.090 (3)	0.065 (3)	−0.030 (2)	−0.021 (2)	−0.005 (2)
C9B	0.0389 (19)	0.056 (2)	0.078 (3)	0.0079 (16)	−0.0175 (18)	−0.021 (2)
C6B	0.053 (2)	0.040 (2)	0.084 (3)	0.0015 (16)	−0.0076 (19)	−0.009 (2)
C8B	0.069 (3)	0.079 (3)	0.064 (3)	0.036 (2)	−0.031 (2)	−0.032 (2)
C15B	0.081 (3)	0.052 (2)	0.052 (2)	0.002 (2)	−0.0035 (19)	−0.0068 (19)
C19A	0.087 (3)	0.048 (2)	0.050 (2)	0.006 (2)	−0.0067 (19)	−0.0074 (18)
C16A	0.139 (4)	0.065 (3)	0.070 (3)	0.020 (3)	−0.061 (3)	−0.017 (2)
C15A	0.101 (3)	0.050 (2)	0.066 (3)	0.019 (2)	−0.031 (2)	−0.019 (2)
C11B	0.086 (3)	0.047 (2)	0.062 (2)	0.008 (2)	−0.022 (2)	−0.0129 (19)
C19B	0.071 (3)	0.055 (2)	0.051 (2)	−0.0111 (19)	−0.0023 (18)	−0.0106 (19)
C16B	0.081 (3)	0.048 (2)	0.068 (3)	−0.001 (2)	0.010 (2)	−0.004 (2)
C7B	0.071 (3)	0.061 (3)	0.062 (3)	0.026 (2)	−0.001 (2)	−0.002 (2)
C17B	0.061 (3)	0.056 (3)	0.087 (3)	−0.0099 (19)	0.006 (2)	−0.023 (2)
C13B	0.070 (3)	0.075 (3)	0.095 (4)	−0.001 (2)	0.009 (2)	−0.009 (3)
C18B	0.081 (3)	0.074 (3)	0.061 (3)	−0.012 (2)	−0.006 (2)	−0.020 (2)
C18A	0.084 (3)	0.045 (2)	0.068 (3)	0.013 (2)	−0.008 (2)	−0.004 (2)
C12B	0.078 (3)	0.062 (3)	0.054 (2)	−0.012 (2)	0.0000 (19)	−0.007 (2)
C13A	0.057 (3)	0.089 (3)	0.079 (3)	0.010 (2)	−0.006 (2)	−0.021 (3)
C5B	0.113 (5)	0.096 (4)	0.160 (6)	0.060 (4)	−0.102 (5)	−0.075 (4)
C12A	0.078 (3)	0.056 (2)	0.051 (2)	0.019 (2)	−0.0197 (19)	−0.019 (2)
C3B	0.065 (3)	0.046 (3)	0.155 (6)	0.001 (2)	−0.034 (3)	0.008 (3)
C17A	0.087 (3)	0.054 (3)	0.076 (3)	0.006 (2)	−0.038 (2)	0.000 (2)
C2B	0.088 (4)	0.076 (3)	0.090 (4)	0.046 (3)	−0.035 (3)	−0.030 (3)
C4B	0.092 (4)	0.126 (5)	0.067 (3)	0.054 (4)	−0.003 (3)	0.024 (3)
C6A	0.0379 (18)	0.048 (2)	0.051 (2)	−0.0018 (15)	−0.0074 (14)	0.0028 (17)
C9A	0.053 (2)	0.047 (2)	0.061 (2)	0.0054 (16)	−0.0079 (17)	0.0093 (18)
C2A	0.058 (2)	0.045 (2)	0.070 (3)	−0.0051 (17)	−0.0093 (19)	0.0036 (19)
C8A	0.070 (3)	0.043 (2)	0.071 (3)	−0.0047 (18)	0.013 (2)	−0.011 (2)
C4A	0.038 (2)	0.059 (2)	0.080 (3)	−0.0057 (16)	−0.0078 (18)	−0.003 (2)
C1A	0.071 (3)	0.061 (3)	0.075 (3)	−0.027 (2)	0.011 (2)	−0.021 (2)

Geometric parameters (Å, º)

Fe2—C5B	2.006 (4)	C5A—H5A	0.93
Fe2—C1B	2.008 (4)	C9B—C8B	1.413 (5)
Fe2—C4B	2.019 (5)	C9B—H10B	0.93
Fe2—C3B	2.030 (4)	C6B—C7B	1.389 (6)
Fe2—C6B	2.031 (4)	C6B—H8B	0.93
Fe2—C9B	2.031 (3)	C8B—C7B	1.403 (6)
Fe2—C10B	2.034 (3)	C8B—H6B	0.93
Fe2—C2B	2.037 (4)	C15B—C16B	1.381 (6)

Fe2—C7B	2.038 (4)	C15B—H15B	0.93
Fe2—C8B	2.041 (4)	C19A—C18A	1.376 (5)
Fe1—C9A	2.022 (3)	C19A—H19A	0.93
Fe1—C5A	2.024 (4)	C16A—C17A	1.368 (6)
Fe1—C10A	2.026 (3)	C16A—C15A	1.385 (5)
Fe1—C1A	2.028 (4)	C16A—H16A	0.93
Fe1—C6A	2.028 (3)	C15A—H15A	0.93
Fe1—C4A	2.038 (3)	C11B—H11C	0.97
Fe1—C8A	2.040 (4)	C11B—H11D	0.97
Fe1—C2A	2.040 (4)	C19B—C18B	1.377 (5)
Fe1—C7A	2.041 (4)	C19B—H19B	0.93
Fe1—C3A	2.044 (4)	C16B—C17B	1.366 (6)
O1—C12A	1.224 (4)	C16B—H16B	0.93
C14A—C19A	1.372 (5)	C7B—H7B	0.93
C14A—C15A	1.374 (5)	C17B—C18B	1.373 (6)
C14A—N1	1.435 (4)	C17B—H17B	0.93
N2—C12B	1.363 (5)	C13B—C12B	1.515 (6)
N2—C14B	1.439 (4)	C13B—H13D	0.96
N2—C11B	1.478 (4)	C13B—H13E	0.96
C10B—C6B	1.417 (5)	C13B—H13F	0.96
C10B—C9B	1.423 (5)	C18B—H18B	0.93
C10B—C11B	1.495 (5)	C18A—C17A	1.366 (6)
N1—C12A	1.359 (5)	C18A—H18A	0.93
N1—C11A	1.478 (4)	C13A—C12A	1.510 (5)
O2—C12B	1.216 (5)	C13A—H13A	0.96
C3A—C4A	1.396 (5)	C13A—H13B	0.96
C3A—C2A	1.402 (5)	C13A—H13C	0.96
C3A—H3A	0.93	C5B—C4B	1.413 (8)
C10A—C6A	1.409 (5)	C5B—H5B	0.93
C10A—C9A	1.420 (5)	C3B—C2B	1.337 (7)
C10A—C11A	1.506 (5)	C3B—C4B	1.347 (8)
C7A—C8A	1.398 (5)	C3B—H3B	0.93
C7A—C6A	1.421 (5)	C17A—H17A	0.93
C7A—H7A	0.93	C2B—H2B	0.93
C1B—C2B	1.357 (7)	C4B—H4B	0.93
C1B—C5B	1.379 (8)	C6A—H6A	0.93
C1B—H1B	0.93	C9A—C8A	1.397 (5)
C14B—C19B	1.369 (5)	C9A—H9A	0.93
C14B—C15B	1.377 (5)	C2A—C1A	1.401 (6)
C11A—H11A	0.97	C2A—H2A	0.93
C11A—H11B	0.97	C8A—H8A	0.93
C5A—C4A	1.406 (6)	C4A—H4A	0.93
C5A—C1A	1.414 (6)	C1A—H1A	0.93

C5B—Fe2—C1B	40.2 (2)	C4A—C5A—H5A	126.2
C5B—Fe2—C4B	41.1 (2)	C1A—C5A—H5A	126.2
C1B—Fe2—C4B	67.4 (2)	Fe1—C5A—H5A	125.4
C5B—Fe2—C3B	66.6 (2)	C8B—C9B—C10B	107.8 (4)

C1B—Fe2—C3B	65.69 (19)	C8B—C9B—Fe2	70.1 (2)
C4B—Fe2—C3B	38.9 (2)	C10B—C9B—Fe2	69.58 (19)
C5B—Fe2—C6B	110.1 (2)	C8B—C9B—H10B	126.1
C1B—Fe2—C6B	114.67 (18)	C10B—C9B—H10B	126.1
C4B—Fe2—C6B	136.1 (3)	Fe2—C9B—H10B	125.8
C3B—Fe2—C6B	174.9 (2)	C7B—C6B—C10B	109.2 (4)
C5B—Fe2—C9B	143.4 (3)	C7B—C6B—Fe2	70.3 (2)
C1B—Fe2—C9B	175.3 (2)	C10B—C6B—Fe2	69.7 (2)
C4B—Fe2—C9B	113.4 (2)	C7B—C6B—H8B	125.4
C3B—Fe2—C9B	111.81 (18)	C10B—C6B—H8B	125.4
C6B—Fe2—C9B	68.21 (15)	Fe2—C6B—H8B	126.2
C5B—Fe2—C10B	112.9 (2)	C7B—C8B—C9B	108.2 (4)
C1B—Fe2—C10B	143.6 (2)	C7B—C8B—Fe2	69.8 (2)
C4B—Fe2—C10B	109.84 (19)	C9B—C8B—Fe2	69.3 (2)
C3B—Fe2—C10B	135.9 (2)	C7B—C8B—H6B	125.9
C6B—Fe2—C10B	40.81 (14)	C9B—C8B—H6B	125.9
C9B—Fe2—C10B	41.00 (13)	Fe2—C8B—H6B	126.6
C5B—Fe2—C2B	66.5 (2)	C14B—C15B—C16B	119.8 (4)
C1B—Fe2—C2B	39.2 (2)	C14B—C15B—H15B	120.1
C4B—Fe2—C2B	65.7 (2)	C16B—C15B—H15B	120.1
C3B—Fe2—C2B	38.4 (2)	C14A—C19A—C18A	120.7 (4)
C6B—Fe2—C2B	144.9 (2)	C14A—C19A—H19A	119.7
C9B—Fe2—C2B	136.39 (19)	C18A—C19A—H19A	119.7
C10B—Fe2—C2B	174.3 (2)	C17A—C16A—C15A	120.9 (4)
C5B—Fe2—C7B	135.2 (3)	C17A—C16A—H16A	119.6
C1B—Fe2—C7B	111.34 (18)	C15A—C16A—H16A	119.6
C4B—Fe2—C7B	175.5 (3)	C14A—C15A—C16A	119.5 (4)
C3B—Fe2—C7B	145.2 (2)	C14A—C15A—H15A	120.2
C6B—Fe2—C7B	39.93 (16)	C16A—C15A—H15A	120.2
C9B—Fe2—C7B	68.19 (16)	N2—C11B—C10B	113.1 (3)
C10B—Fe2—C7B	68.36 (15)	N2—C11B—H11C	109
C2B—Fe2—C7B	116.37 (19)	C10B—C11B—H11C	109
C5B—Fe2—C8B	175.0 (3)	N2—C11B—H11D	109
C1B—Fe2—C8B	136.1 (2)	C10B—C11B—H11D	109
C4B—Fe2—C8B	143.6 (3)	H11C—C11B—H11D	107.8
C3B—Fe2—C8B	116.1 (2)	C14B—C19B—C18B	119.3 (4)
C6B—Fe2—C8B	67.48 (17)	C14B—C19B—H19B	120.3
C9B—Fe2—C8B	40.60 (15)	C18B—C19B—H19B	120.3
C10B—Fe2—C8B	68.47 (14)	C17B—C16B—C15B	120.3 (4)
C2B—Fe2—C8B	112.73 (17)	C17B—C16B—H16B	119.8
C7B—Fe2—C8B	40.24 (17)	C15B—C16B—H16B	119.8
C9A—Fe1—C5A	107.14 (17)	C6B—C7B—C8B	108.2 (4)
C9A—Fe1—C10A	41.06 (13)	C6B—C7B—Fe2	69.8 (2)
C5A—Fe1—C10A	114.86 (16)	C8B—C7B—Fe2	70.0 (2)
C9A—Fe1—C1A	128.96 (18)	C6B—C7B—H7B	125.9
C5A—Fe1—C1A	40.85 (17)	C8B—C7B—H7B	125.9
C10A—Fe1—C1A	106.73 (15)	Fe2—C7B—H7B	125.9
C9A—Fe1—C6A	68.28 (14)	C16B—C17B—C18B	119.3 (4)

C5A—Fe1—C6A	148.24 (17)	C16B—C17B—H17B	120.3
C10A—Fe1—C6A	40.66 (13)	C18B—C17B—H17B	120.3
C1A—Fe1—C6A	116.23 (16)	C12B—C13B—H13D	109.5
C9A—Fe1—C4A	116.56 (15)	C12B—C13B—H13E	109.5
C5A—Fe1—C4A	40.48 (16)	H13D—C13B—H13E	109.5
C10A—Fe1—C4A	148.34 (15)	C12B—C13B—H13F	109.5
C1A—Fe1—C4A	68.09 (16)	H13D—C13B—H13F	109.5
C6A—Fe1—C4A	170.28 (15)	H13E—C13B—H13F	109.5
C9A—Fe1—C8A	40.21 (15)	C17B—C18B—C19B	121.0 (4)
C5A—Fe1—C8A	129.55 (19)	C17B—C18B—H18B	119.5
C10A—Fe1—C8A	68.57 (14)	C19B—C18B—H18B	119.5
C1A—Fe1—C8A	167.65 (19)	C17A—C18A—C19A	120.2 (4)
C6A—Fe1—C8A	68.23 (15)	C17A—C18A—H18A	119.9
C4A—Fe1—C8A	109.49 (16)	C19A—C18A—H18A	119.9
C9A—Fe1—C2A	167.78 (16)	O2—C12B—N2	121.2 (4)
C5A—Fe1—C2A	68.18 (17)	O2—C12B—C13B	121.8 (4)
C10A—Fe1—C2A	129.41 (14)	N2—C12B—C13B	117.1 (4)
C1A—Fe1—C2A	40.30 (16)	C12A—C13A—H13A	109.5
C6A—Fe1—C2A	109.33 (15)	C12A—C13A—H13B	109.5
C4A—Fe1—C2A	67.81 (15)	H13A—C13A—H13B	109.5
C8A—Fe1—C2A	151.25 (17)	C12A—C13A—H13C	109.5
C9A—Fe1—C7A	67.68 (16)	H13A—C13A—H13C	109.5
C5A—Fe1—C7A	168.53 (18)	H13B—C13A—H13C	109.5
C10A—Fe1—C7A	68.54 (14)	C1B—C5B—C4B	106.4 (5)
C1A—Fe1—C7A	150.29 (18)	C1B—C5B—Fe2	70.0 (3)
C6A—Fe1—C7A	40.89 (14)	C4B—C5B—Fe2	69.9 (3)
C4A—Fe1—C7A	131.44 (16)	C1B—C5B—H5B	126.8
C8A—Fe1—C7A	40.06 (16)	C4B—C5B—H5B	126.8
C2A—Fe1—C7A	118.96 (16)	Fe2—C5B—H5B	124.9
C9A—Fe1—C3A	149.96 (15)	O1—C12A—N1	121.0 (4)
C5A—Fe1—C3A	67.63 (16)	O1—C12A—C13A	121.3 (4)
C10A—Fe1—C3A	168.82 (14)	N1—C12A—C13A	117.7 (3)
C1A—Fe1—C3A	67.51 (16)	C2B—C3B—C4B	110.1 (5)
C6A—Fe1—C3A	132.00 (14)	C2B—C3B—Fe2	71.1 (3)
C4A—Fe1—C3A	40.00 (14)	C4B—C3B—Fe2	70.1 (3)
C8A—Fe1—C3A	119.04 (16)	C2B—C3B—H3B	124.9
C2A—Fe1—C3A	40.14 (14)	C4B—C3B—H3B	124.9
C7A—Fe1—C3A	111.33 (15)	Fe2—C3B—H3B	125.4
C19A—C14A—C15A	119.4 (3)	C18A—C17A—C16A	119.3 (4)
C19A—C14A—N1	120.8 (3)	C18A—C17A—H17A	120.3
C15A—C14A—N1	119.8 (3)	C16A—C17A—H17A	120.3
C12B—N2—C14B	124.7 (3)	C3B—C2B—C1B	108.7 (5)
C12B—N2—C11B	118.9 (3)	C3B—C2B—Fe2	70.5 (3)
C14B—N2—C11B	116.2 (3)	C1B—C2B—Fe2	69.2 (3)
C6B—C10B—C9B	106.6 (3)	C3B—C2B—H2B	125.6
C6B—C10B—C11B	127.5 (3)	C1B—C2B—H2B	125.6
C9B—C10B—C11B	125.8 (3)	Fe2—C2B—H2B	126.2
C6B—C10B—Fe2	69.5 (2)	C3B—C4B—C5B	106.7 (5)

C9B—C10B—Fe2	69.42 (19)	C3B—C4B—Fe2	71.0 (3)
C11B—C10B—Fe2	125.9 (2)	C5B—C4B—Fe2	68.9 (3)
C12A—N1—C14A	124.2 (3)	C3B—C4B—H4B	126.6
C12A—N1—C11A	118.7 (3)	C5B—C4B—H4B	126.6
C14A—N1—C11A	116.9 (3)	Fe2—C4B—H4B	125
C4A—C3A—C2A	108.8 (4)	C10A—C6A—C7A	108.0 (3)
C4A—C3A—Fe1	69.8 (2)	C10A—C6A—Fe1	69.60 (19)
C2A—C3A—Fe1	69.8 (2)	C7A—C6A—Fe1	70.0 (2)
C4A—C3A—H3A	125.6	C10A—C6A—H6A	126
C2A—C3A—H3A	125.6	C7A—C6A—H6A	126
Fe1—C3A—H3A	126.4	Fe1—C6A—H6A	126
C6A—C10A—C9A	107.0 (3)	C8A—C9A—C10A	108.8 (3)
C6A—C10A—C11A	126.2 (3)	C8A—C9A—Fe1	70.6 (2)
C9A—C10A—C11A	126.8 (3)	C10A—C9A—Fe1	69.61 (19)
C6A—C10A—Fe1	69.74 (18)	C8A—C9A—H9A	125.6
C9A—C10A—Fe1	69.32 (19)	C10A—C9A—H9A	125.6
C11A—C10A—Fe1	124.6 (2)	Fe1—C9A—H9A	125.8
C8A—C7A—C6A	108.1 (3)	C1A—C2A—C3A	107.6 (3)
C8A—C7A—Fe1	70.0 (2)	C1A—C2A—Fe1	69.4 (2)
C6A—C7A—Fe1	69.1 (2)	C3A—C2A—Fe1	70.0 (2)
C8A—C7A—H7A	126	C1A—C2A—H2A	126.2
C6A—C7A—H7A	126	C3A—C2A—H2A	126.2
Fe1—C7A—H7A	126.6	Fe1—C2A—H2A	126
C2B—C1B—C5B	108.1 (5)	C9A—C8A—C7A	108.1 (3)
C2B—C1B—Fe2	71.6 (3)	C9A—C8A—Fe1	69.2 (2)
C5B—C1B—Fe2	69.8 (3)	C7A—C8A—Fe1	70.0 (2)
C2B—C1B—H1B	126	C9A—C8A—H8A	125.9
C5B—C1B—H1B	126	C7A—C8A—H8A	125.9
Fe2—C1B—H1B	124.3	Fe1—C8A—H8A	126.5
C19B—C14B—C15B	120.2 (4)	C3A—C4A—C5A	107.8 (4)
C19B—C14B—N2	119.4 (3)	C3A—C4A—Fe1	70.2 (2)
C15B—C14B—N2	120.3 (3)	C5A—C4A—Fe1	69.2 (2)
N1—C11A—C10A	113.1 (3)	C3A—C4A—H4A	126.1
N1—C11A—H11A	109	C5A—C4A—H4A	126.1
C10A—C11A—H11A	109	Fe1—C4A—H4A	126.1
N1—C11A—H11B	109	C2A—C1A—C5A	108.0 (4)
C10A—C11A—H11B	109	C2A—C1A—Fe1	70.3 (2)
H11A—C11A—H11B	107.8	C5A—C1A—Fe1	69.4 (2)
C4A—C5A—C1A	107.7 (4)	C2A—C1A—H1A	126
C4A—C5A—Fe1	70.3 (2)	C5A—C1A—H1A	126
C1A—C5A—Fe1	69.7 (2)	Fe1—C1A—H1A	125.8

C19A—C14A—N1—C12A	110.5 (4)	C2B—C1B—C5B—C4B	−0.8 (5)
C15A—C14A—N1—C12A	−71.6 (5)	Fe2—C1B—C5B—C4B	60.8 (3)
C19A—C14A—N1—C11A	−75.3 (4)	C2B—C1B—C5B—Fe2	−61.7 (3)
C15A—C14A—N1—C11A	102.6 (4)	C14A—N1—C12A—O1	173.5 (3)
C12B—N2—C14B—C19B	84.9 (5)	C11A—N1—C12A—O1	−0.6 (5)
C11B—N2—C14B—C19B	−89.9 (4)	C14A—N1—C12A—C13A	−7.0 (5)

C12B—N2—C14B—C15B	−98.1 (4)	C11A—N1—C12A—C13A	178.9 (3)
C11B—N2—C14B—C15B	87.2 (4)	C19A—C18A—C17A—C16A	0.3 (7)
C12A—N1—C11A—C10A	−92.1 (4)	C15A—C16A—C17A—C18A	−1.6 (8)
C14A—N1—C11A—C10A	93.3 (4)	C4B—C3B—C2B—C1B	−0.6 (5)
C6A—C10A—C11A—N1	93.3 (4)	Fe2—C3B—C2B—C1B	58.9 (3)
C9A—C10A—C11A—N1	−88.7 (4)	C4B—C3B—C2B—Fe2	−59.5 (3)
Fe1—C10A—C11A—N1	−177.6 (2)	C5B—C1B—C2B—C3B	0.9 (5)
C6B—C10B—C9B—C8B	0.0 (4)	Fe2—C1B—C2B—C3B	−59.7 (3)
C11B—C10B—C9B—C8B	−180.0 (3)	C5B—C1B—C2B—Fe2	60.6 (3)
Fe2—C10B—C9B—C8B	−59.9 (2)	C2B—C3B—C4B—C5B	0.1 (5)
C6B—C10B—C9B—Fe2	59.8 (2)	Fe2—C3B—C4B—C5B	−60.0 (3)
C11B—C10B—C9B—Fe2	−120.1 (3)	C2B—C3B—C4B—Fe2	60.1 (3)
C9B—C10B—C6B—C7B	−0.4 (4)	C1B—C5B—C4B—C3B	0.5 (5)
C11B—C10B—C6B—C7B	179.6 (3)	Fe2—C5B—C4B—C3B	61.3 (3)
Fe2—C10B—C6B—C7B	59.4 (3)	C1B—C5B—C4B—Fe2	−60.8 (3)
C9B—C10B—C6B—Fe2	−59.8 (2)	C9A—C10A—C6A—C7A	0.1 (4)
C11B—C10B—C6B—Fe2	120.2 (3)	C11A—C10A—C6A—C7A	178.4 (3)
C10B—C9B—C8B—C7B	0.4 (4)	Fe1—C10A—C6A—C7A	59.7 (2)
Fe2—C9B—C8B—C7B	−59.1 (3)	C9A—C10A—C6A—Fe1	−59.6 (2)
C10B—C9B—C8B—Fe2	59.6 (2)	C11A—C10A—C6A—Fe1	118.7 (3)
C19B—C14B—C15B—C16B	0.9 (6)	C8A—C7A—C6A—C10A	−0.1 (4)
N2—C14B—C15B—C16B	−176.2 (4)	Fe1—C7A—C6A—C10A	−59.4 (2)
C15A—C14A—C19A—C18A	−1.7 (6)	C8A—C7A—C6A—Fe1	59.3 (2)
N1—C14A—C19A—C18A	176.3 (4)	C6A—C10A—C9A—C8A	0.0 (4)
C19A—C14A—C15A—C16A	0.3 (7)	C11A—C10A—C9A—C8A	−178.3 (3)
N1—C14A—C15A—C16A	−177.7 (4)	Fe1—C10A—C9A—C8A	−59.9 (3)
C17A—C16A—C15A—C14A	1.3 (8)	C6A—C10A—C9A—Fe1	59.9 (2)
C12B—N2—C11B—C10B	91.5 (4)	C11A—C10A—C9A—Fe1	−118.4 (3)
C14B—N2—C11B—C10B	−93.3 (4)	C4A—C3A—C2A—C1A	0.4 (4)
C6B—C10B—C11B—N2	82.3 (5)	Fe1—C3A—C2A—C1A	59.4 (2)
C9B—C10B—C11B—N2	−97.7 (4)	C4A—C3A—C2A—Fe1	−59.1 (2)
Fe2—C10B—C11B—N2	173.0 (2)	C10A—C9A—C8A—C7A	−0.1 (4)
C15B—C14B—C19B—C18B	0.3 (6)	Fe1—C9A—C8A—C7A	−59.4 (3)
N2—C14B—C19B—C18B	177.3 (4)	C10A—C9A—C8A—Fe1	59.3 (2)
C14B—C15B—C16B—C17B	−1.1 (6)	C6A—C7A—C8A—C9A	0.1 (4)
C10B—C6B—C7B—C8B	0.7 (4)	Fe1—C7A—C8A—C9A	58.9 (3)
Fe2—C6B—C7B—C8B	59.7 (3)	C6A—C7A—C8A—Fe1	−58.8 (2)
C10B—C6B—C7B—Fe2	−59.0 (2)	C2A—C3A—C4A—C5A	−0.2 (4)
C9B—C8B—C7B—C6B	−0.7 (4)	Fe1—C3A—C4A—C5A	−59.2 (3)
Fe2—C8B—C7B—C6B	−59.5 (3)	C2A—C3A—C4A—Fe1	59.1 (2)
C9B—C8B—C7B—Fe2	58.9 (3)	C1A—C5A—C4A—C3A	−0.1 (4)
C15B—C16B—C17B—C18B	0.2 (6)	Fe1—C5A—C4A—C3A	59.8 (3)
C16B—C17B—C18B—C19B	0.9 (7)	C1A—C5A—C4A—Fe1	−59.9 (3)
C14B—C19B—C18B—C17B	−1.2 (6)	C3A—C2A—C1A—C5A	−0.4 (4)
C14A—C19A—C18A—C17A	1.4 (7)	Fe1—C2A—C1A—C5A	59.4 (3)
C14B—N2—C12B—O2	−177.5 (4)	C3A—C2A—C1A—Fe1	−59.8 (2)
C11B—N2—C12B—O2	−2.9 (6)	C4A—C5A—C1A—C2A	0.3 (4)
C14B—N2—C12B—C13B	2.5 (6)	Fe1—C5A—C1A—C2A	−60.0 (3)

C11B—N2—C12B—C13B	177.2 (3)	C4A—C5A—C1A—Fe1	60.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15*A*—H15*A*···O1^{i}	0.93	2.56	3.456 (5)	162
C19*B*—H19*B*···O2^{ii}	0.93	2.55	3.421 (5)	157
C15*A*—H15*A*···O1^{i}	0.93	2.56	3.456 (5)	162
C19*B*—H19*B*···O2^{ii}	0.93	2.55	3.421 (5)	157

Symmetry codes: (i) −*x*−1, −*y*+2, −*z*+1; (ii) −*x*, −*y*+1, −*z*+2.