

## 5-Chloro-2-ferrocenylbenzo[d]oxazole

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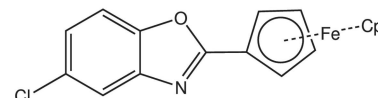
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

The asymmetric unit of the title compound,  $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{12}\text{H}_7\text{ClNO})]$ , consists of one ferrocenyl group bonded to chlorobenzo[d]oxazole. The conformation of the ferrocenyl moiety is slightly away from eclipsed. The bond angles between the 5-chloro-benzoxazole and ferrocenyl fragments are  $\text{N}-\text{C}-\text{C} = 127.4 (7)^\circ$  and  $\text{O}-\text{C}-\text{C} = 116.8 (7)^\circ$ . The benzo[d]oxazole ring is planar (r.m.s. deviation =  $0.0042 \text{ \AA}$ ) and makes an angle of  $11.3 (4)^\circ$  with the cyclopentadienyl ring attached to it. The crystal packing is characterized by intermolecular  $\pi-\pi$  contacts, resulting in chain formation along the *b*-axis direction. The centroid-to-centroid distance between the six- and five-membered rings is  $3.650 (5) \text{ \AA}$ . Together with a  $\text{C}-\text{H}\cdots\pi$  interaction, these intermolecular contacts form laminar arrays along the *ac* plane.

### 3D view



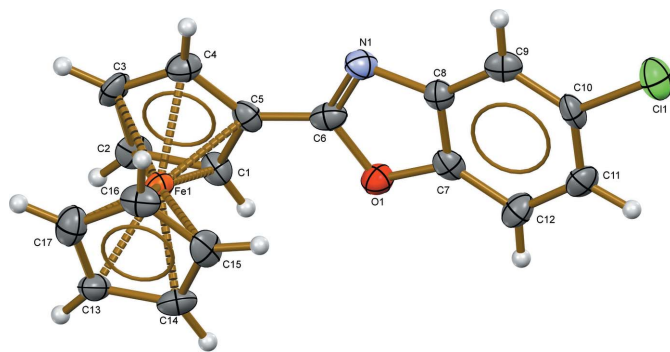
### Chemical scheme



### Structure description

Benzoxazoles are among the most important compounds in heterocyclic compounds. They exhibit remarkable pharmacological activities, are used as building blocks for biochemical and pharmaceutical agents (Singh *et al.*, 2015), including antibiotic, antimicrobial, antivirals, dyes, fluorescent brightening agents, biomarkers, biosensors and fluorescent materials (Zhang *et al.*, 2017). The major strategy for the synthesis of benzoxazoles (Boyd *et al.*, 2002) is the condensation of carboxylic acids and their derivatives with 2-aminophenoles, but this often requires harsh reaction conditions (high reaction temperature and use of acidic activators and oxidants).

It is known that ferrocene derivatives (Togni & Hayashi, 1995) exhibit important functional derivatives, which are useful in medicinal as well as in synthetic fields (Larik *et al.*, 2017). The incorporation of a ferrocene entity can significantly improve the biological activity of molecules (Klimova *et al.*, 2012). Many drugs contain ferrocene moieties in

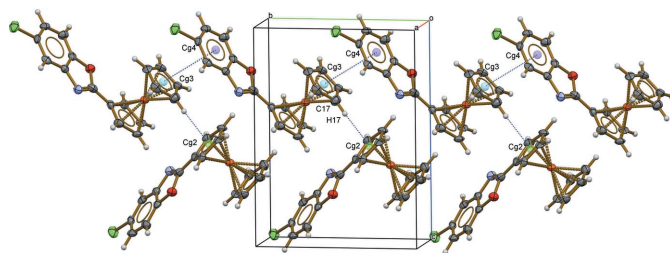


**Figure 1**  
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 60% probability level.

their structures, such as ferrocifen, tamoxifen (Top *et al.*, 2003; Jaouen *et al.*, 2015) and ferroquine, which are excellent anticancer and antimalarial agents (Dubar *et al.*, 2008).

In this context, it is proposed that due to the synergy between a benzoxazole and a ferrocene unit present in a molecule, it should exhibit an important biological activity. We present here a continuation of this work, we present here the synthesis of 2-ferrocenylbenzoxazoles and the crystal structure of 5-chloro-2-ferrocenylbenzo[*d*]oxazole. The synthesis of this compound was done by reaction of diferrocenylcyclopropenyl cations (Klimova *et al.*, 2003) with aminoalcohols in the presence of triethylamine, obtaining good yields (Sánchez *et al.*, 2018).

The asymmetric unit of the title compound (Fig. 1) consist of one ferrocenyl bonded through the C5 atom to 5-chlorobenzo[*d*]oxazole. All bond lengths and angles are in the range observed for ferrocenyl and aromatic rings, and in the same way, the bond lengths C6=N1 = 1.297 (10), C7–O1 = 1.381 (9) and C10–Cl1 = 1.751 (8) Å correspond to literature reports (Su *et al.*, 2018; Liu *et al.*, 2017). The conformation of the ferrocenyl moiety is slightly away from eclipsed. The bond angles between the 5-chloro-benzoxazole and ferrocenyl fragments are N1–C6–C5 = 127.4 (7)° and O1–C6–C5 = 116.8 (7)°. The five- and six-membered rings of the 5-chlorobenzo[*d*]oxazole fragment are coplanar with an r.m.s. deviation for the fitted atoms of 0.0042 Å [equation plane:  $-2.42(1)x + 6.79(1)y + 7.16(2)z = 7.60(2)$ ]. However, there is a slight deviation from the coplanarity with the 5-chloro-



**Figure 2**  
Crystal packing of 5-chloro-2-ferrocenylbenzo[*d*]oxazole showing the short contacts of type  $\pi$ – $\pi$  and C–H $\cdots\pi$ .

benzo[*d*]oxazole and the five-membered C1–C5 rings making an angle of 11.3 (4)°.

In the crystal packing (Fig. 2), there are intermolecular  $\pi$ – $\pi$  and C–H $\cdots\pi$  contacts. The centroids Cg3 of the five-membered ring C13–C17 of the ferrocenyl group and Cg4 of the six-membered ring C7–C12 of 5-chlorobenzo[*d*]oxazole establish a weak intermolecular  $\pi$ – $\pi$  interaction [Cg3 $\cdots$ Cg4<sup>i</sup> = 3.650 (5) Å; symmetry code: (i)  $x, y - 1, z$ ], resulting in chain formation along the *b*-axis direction. On the other hand, an intermolecular interaction C17–H17 $\cdots$ Cg2<sup>ii</sup> [Cg2 is the centroid of ring C1–C5; H17 $\cdots$ Cg2 = 3.322 Å; symmetry code: (ii)  $-x + 1, y - \frac{1}{2}, -z + 1$ ] of type C–H $\cdots\pi$  is present. All these intermolecular contacts form a laminar array along the *ac* plane.

### Synthesis and crystallization

2-Amino-4-chlorophenol (5 mmol) and Et<sub>3</sub>N (1.0 ml) were added while stirring to a solution of 1-morpholine-2,3-diferrocenylcyclopropenium tetrafluoroborate (4 mmol) (Klimova *et al.* 2005) in dry acetonitrile (70 ml). After stirring for 6 h at 348 K, the solvents were removed *in vacuo* and the residue was dissolved in dichloromethane (30 ml). The solution was mixed with Al<sub>2</sub>O<sub>3</sub> (activity III) (20 g) and the solvent was evaporated in air. This material was placed on the top of a column with Al<sub>2</sub>O<sub>3</sub> (the height of alumina was *ca* 20 cm) and the elution was performed first with hexane and then with hexane - ether (3:1) and hexane - dichloromethane (4:1) to give the title compound (yield 30%, orange–brown crystals, m.p. 421–422 K). <sup>1</sup>H NMR [400 MHz, CDCl<sub>3</sub>,  $\delta$  (p.p.m.)]: 4.18 (*s*, 5H, C<sub>5</sub>H<sub>5</sub>), 4.53 (*m*, 2H, C<sub>5</sub>H<sub>4</sub>), 5.07 (*m*, 2H, C<sub>5</sub>H<sub>4</sub>), 7.27 (*dd*, *J* = 2.1, 8.4 Hz, 1H, C<sub>6</sub>H<sub>3</sub>), 7.43 (*d*, *J* = 8.4 Hz, 1H, C<sub>6</sub>H<sub>3</sub>), 7.64 (*d*, *J* = 2.1 Hz, 1H, C<sub>6</sub>H<sub>3</sub>). <sup>13</sup>C NMR [100 MHz, CDCl<sub>3</sub>,  $\delta$  (p.p.m.)]: 70.58 (C<sub>5</sub>H<sub>5</sub>), 69.25, 71.71 (C<sub>5</sub>H<sub>4</sub>), 80.85 (C<sub>ipso</sub>Fc), 114.83, 127.04, 127.87 (C<sub>6</sub>H<sub>3</sub>), 131.29, 145.27, 163.23 (3 C). MS (EI, 70 eV): *m/z* 337 [*M*]<sup>+</sup>. Analysis calculated for C<sub>17</sub>H<sub>12</sub>ClFeNO: C, 60.48; H, 3.58; N, 4.15. Found: C, 60.47; H, 3.52; N, 4.27%.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

### Acknowledgements

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### References

Agilent (2013). *CrysAlis PRO* and *CrysAlis RED*. Agilent Technologies, Yarnton, England.

**Table 1**  
Experimental details.

Crystal data	
Chemical formula	[Fe(C <sub>5</sub> H <sub>5</sub> )(C <sub>12</sub> H <sub>7</sub> ClNO)]
<i>M</i> <sub>r</sub>	337.58
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub>
Temperature (K)	130
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.7854 (7), 9.2974 (11), 12.6443 (12)
$\beta$ (°)	94.217 (10)
<i>V</i> (Å <sup>3</sup> )	678.29 (13)
<i>Z</i>	2
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	1.30
Crystal size (mm)	0.18 × 0.06 × 0.04
Data collection	
Diffractometer	Agilent Xcalibur Atlas Gemini
Absorption correction	Analytical ( <i>CrysAlis RED</i> ; Agilent, 2013)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.89, 0.956
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	3384, 2001, 1782
<i>R</i> <sub>int</sub>	0.045
( $\sin \theta/\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.602
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.047, 0.114, 1.08
No. of reflections	2001
No. of parameters	190
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	1.02, -0.49
Absolute structure	Flack <i>x</i> determined using 562 quotients [( <i>I</i> <sup>+</sup> ) - ( <i>I</i> <sup>-</sup> )] / [( <i>I</i> <sup>+</sup> ) + ( <i>I</i> <sup>-</sup> )] (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.01 (3)

Computer programs: *CrysAlis PRO* (Agilent, 2013), *CrysAlis PRO*; Agilent, 2013, *CrysAlis RED* (Agilent, 2013), *SHELXS2018* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006).

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## full crystallographic data

*IUCrData* (2019), 4, x191096 [https://doi.org/10.1107/S2414314619010964]

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*Crystal data*

[Fe(C<sub>5</sub>H<sub>5</sub>)(C<sub>12</sub>H<sub>7</sub>CINO)]

$M_r = 337.58$

Monoclinic,  $P2_1$

Hall symbol: P 2yb

$a = 5.7854$  (7) Å

$b = 9.2974$  (11) Å

$c = 12.6443$  (12) Å

$\beta = 94.217$  (10)°

$V = 678.29$  (13) Å<sup>3</sup>

$Z = 2$

$F(000) = 344$

$D_x = 1.653$  Mg m<sup>-3</sup>

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

Cell parameters from 1067 reflections

$\theta = 4.1$ – $27.7$ °

$\mu = 1.30$  mm<sup>-1</sup>

$T = 130$  K

Prism, brown

$0.18 \times 0.06 \times 0.04$  mm

*Data collection*

Agilent Xcalibur Atlas Gemini  
diffractometer

Graphite monochromator

Detector resolution: 10.4685 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: analytical

(*CrysAlis RED*; Agilent, 2013)

$T_{\min} = 0.89$ ,  $T_{\max} = 0.956$

3384 measured reflections

2001 independent reflections

1782 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\max} = 25.3$ °,  $\theta_{\min} = 3.5$ °

$h = -6 \rightarrow 6$

$k = -8 \rightarrow 11$

$l = -14 \rightarrow 15$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.114$

$S = 1.08$

2001 reflections

190 parameters

1 restraint

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2]$

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

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

$\Delta\rho_{\max} = 1.02$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.49$  e Å<sup>-3</sup>

Absolute structure: Flack  $x$  determined using

562 quotients  $[(I^-)-(I)]/[(I^+)+(I)]$  (Parsons et al.,  
2013)

Absolute structure parameter: 0.01 (3)

*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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3847 (12)	0.8652 (9)	0.3871 (7)	0.0214 (18)
H1	0.247272	0.888213	0.344774	0.026*
C2	0.4058 (13)	0.7612 (9)	0.4687 (6)	0.024 (2)
H2	0.285423	0.701615	0.491262	0.028*
C3	0.6407 (14)	0.7623 (9)	0.5108 (7)	0.026 (2)
H3	0.703353	0.702801	0.566885	0.031*
C4	0.7664 (13)	0.8653 (10)	0.4566 (7)	0.0246 (19)
H4	0.926355	0.887431	0.469155	0.03*
C5	0.6079 (13)	0.9296 (9)	0.3797 (7)	0.0213 (18)
C6	0.6662 (13)	1.0362 (9)	0.3026 (7)	0.0243 (19)
C7	0.6049 (13)	1.1657 (8)	0.1601 (6)	0.0213 (18)
C8	0.8238 (12)	1.1923 (9)	0.2083 (6)	0.0201 (18)
C9	0.9673 (13)	1.2921 (8)	0.1624 (7)	0.0236 (19)
H9	1.118427	1.31383	0.192706	0.028*
C10	0.8763 (13)	1.3570 (9)	0.0706 (7)	0.0228 (18)
C11	0.6569 (13)	1.3292 (9)	0.0229 (6)	0.0247 (19)
H11	0.604232	1.378095	-0.040318	0.03*
C12	0.5138 (12)	1.2289 (11)	0.0685 (6)	0.0255 (18)
H12	0.363378	1.206041	0.037843	0.031*
C13	0.5383 (13)	0.5194 (9)	0.2913 (6)	0.0240 (19)
H13	0.413364	0.461252	0.310905	0.029*
C14	0.5257 (15)	0.6234 (9)	0.2105 (7)	0.027 (2)
H14	0.391541	0.647201	0.166087	0.033*
C15	0.7489 (13)	0.6867 (9)	0.2066 (6)	0.026 (2)
H15	0.790132	0.760485	0.159482	0.032*
C16	0.8978 (15)	0.6201 (9)	0.2854 (7)	0.028 (2)
H16	1.057646	0.640494	0.300784	0.033*
C17	0.7634 (15)	0.5156 (10)	0.3380 (7)	0.031 (2)
H17	0.818626	0.454729	0.394737	0.037*
Cl1	1.0453 (4)	1.4841 (2)	0.0092 (2)	0.0328 (6)
Fe1	0.62694 (17)	0.71553 (12)	0.35316 (8)	0.0194 (3)
N1	0.8578 (11)	1.1084 (7)	0.3008 (5)	0.0229 (16)
O1	0.5007 (9)	1.0647 (6)	0.2210 (4)	0.0235 (13)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.019 (4)	0.020 (4)	0.026 (5)	0.001 (3)	0.006 (3)	-0.001 (4)
C2	0.026 (4)	0.031 (5)	0.015 (4)	0.000 (3)	0.014 (3)	-0.005 (4)
C3	0.035 (5)	0.032 (5)	0.011 (4)	0.005 (4)	0.001 (3)	0.002 (3)
C4	0.021 (4)	0.031 (5)	0.022 (4)	-0.003 (4)	0.001 (4)	-0.002 (4)
C5	0.025 (4)	0.016 (4)	0.024 (5)	0.000 (3)	0.006 (3)	-0.004 (4)
C6	0.023 (4)	0.028 (5)	0.022 (5)	0.002 (4)	-0.001 (4)	-0.007 (4)
C7	0.026 (4)	0.019 (4)	0.020 (4)	-0.001 (3)	0.010 (3)	-0.005 (3)
C8	0.022 (3)	0.019 (5)	0.020 (4)	0.002 (3)	0.004 (3)	-0.002 (4)

C9	0.022 (4)	0.027 (5)	0.022 (5)	0.003 (4)	0.006 (3)	-0.008 (4)
C10	0.031 (4)	0.014 (4)	0.024 (5)	-0.003 (4)	0.011 (4)	0.001 (4)
C11	0.030 (4)	0.030 (5)	0.014 (4)	0.000 (4)	0.004 (3)	-0.001 (4)
C12	0.024 (4)	0.029 (5)	0.023 (4)	0.008 (4)	0.000 (3)	0.002 (5)
C13	0.026 (4)	0.027 (5)	0.019 (5)	-0.008 (4)	0.000 (3)	-0.002 (4)
C14	0.027 (4)	0.034 (5)	0.020 (4)	-0.002 (4)	-0.003 (4)	-0.008 (4)
C15	0.034 (4)	0.029 (6)	0.018 (4)	-0.006 (4)	0.015 (3)	0.001 (4)
C16	0.021 (4)	0.029 (5)	0.033 (5)	0.004 (3)	0.001 (4)	-0.009 (4)
C17	0.036 (5)	0.028 (5)	0.029 (5)	0.008 (4)	0.004 (4)	0.004 (4)
Cl1	0.0360 (13)	0.0284 (13)	0.0354 (13)	-0.0030 (10)	0.0122 (11)	0.0046 (11)
Fe1	0.0205 (5)	0.0224 (6)	0.0156 (5)	-0.0004 (6)	0.0022 (4)	-0.0001 (6)
N1	0.022 (4)	0.026 (4)	0.022 (4)	-0.006 (3)	0.003 (3)	-0.001 (3)
O1	0.021 (3)	0.027 (3)	0.023 (3)	-0.001 (2)	0.001 (2)	0.001 (3)

*Geometric parameters (Å, °)*

C1—C2	1.412 (12)	C9—C10	1.378 (11)
C1—C5	1.433 (11)	C9—H9	0.95
C1—Fe1	2.042 (8)	C10—C11	1.389 (10)
C1—H1	0.95	C10—Cl1	1.751 (8)
C2—C3	1.423 (10)	C11—C12	1.399 (12)
C2—Fe1	2.056 (8)	C11—H11	0.95
C2—H2	0.95	C12—H12	0.95
C3—C4	1.410 (12)	C13—C17	1.390 (11)
C3—Fe1	2.036 (8)	C13—C14	1.405 (11)
C3—H3	0.95	C13—Fe1	2.035 (8)
C4—C5	1.419 (11)	C13—H13	0.95
C4—Fe1	2.036 (8)	C14—C15	1.423 (11)
C4—H4	0.95	C14—Fe1	2.044 (8)
C5—C6	1.446 (12)	C14—H14	0.95
C5—Fe1	2.023 (8)	C15—C16	1.412 (11)
C6—N1	1.297 (10)	C15—Fe1	2.049 (8)
C6—O1	1.381 (9)	C15—H15	0.95
C7—C12	1.370 (11)	C16—C17	1.438 (13)
C7—O1	1.381 (9)	C16—Fe1	2.044 (9)
C7—C8	1.387 (10)	C16—H16	0.95
C8—C9	1.400 (12)	C17—Fe1	2.034 (9)
C8—N1	1.408 (10)	C17—H17	0.95
C2—C1—C5	107.7 (7)	C16—C15—Fe1	69.6 (5)
C2—C1—Fe1	70.4 (4)	C14—C15—Fe1	69.5 (5)
C5—C1—Fe1	68.6 (4)	C16—C15—H15	126.2
C2—C1—H1	126.1	C14—C15—H15	126.2
C5—C1—H1	126.1	Fe1—C15—H15	126.3
Fe1—C1—H1	126.4	C15—C16—C17	107.5 (7)
C1—C2—C3	107.3 (7)	C15—C16—Fe1	70.0 (5)
C1—C2—Fe1	69.3 (5)	C17—C16—Fe1	69.0 (5)
C3—C2—Fe1	68.9 (5)	C15—C16—H16	126.3

C1—C2—H2	126.4	C17—C16—H16	126.3
C3—C2—H2	126.4	Fe1—C16—H16	126.3
Fe1—C2—H2	126.9	C13—C17—C16	107.9 (7)
C4—C3—C2	109.6 (7)	C13—C17—Fe1	70.0 (5)
C4—C3—Fe1	69.7 (5)	C16—C17—Fe1	69.7 (5)
C2—C3—Fe1	70.4 (4)	C13—C17—H17	126
C4—C3—H3	125.2	C16—C17—H17	126
C2—C3—H3	125.2	Fe1—C17—H17	125.8
Fe1—C3—H3	126.3	C5—Fe1—C17	160.2 (3)
C3—C4—C5	106.8 (7)	C5—Fe1—C13	158.5 (3)
C3—C4—Fe1	69.7 (5)	C17—Fe1—C13	40.0 (3)
C5—C4—Fe1	69.0 (4)	C5—Fe1—C4	40.9 (3)
C3—C4—H4	126.6	C17—Fe1—C4	123.2 (3)
C5—C4—H4	126.6	C13—Fe1—C4	159.5 (3)
Fe1—C4—H4	126.2	C5—Fe1—C3	68.0 (3)
C4—C5—C1	108.6 (7)	C17—Fe1—C3	107.4 (3)
C4—C5—C6	125.4 (7)	C13—Fe1—C3	123.9 (3)
C1—C5—C6	125.9 (7)	C4—Fe1—C3	40.5 (3)
C4—C5—Fe1	70.0 (5)	C5—Fe1—C1	41.3 (3)
C1—C5—Fe1	70.1 (5)	C17—Fe1—C1	156.8 (3)
C6—C5—Fe1	123.0 (6)	C13—Fe1—C1	122.3 (3)
N1—C6—O1	115.7 (7)	C4—Fe1—C1	69.2 (3)
N1—C6—C5	127.4 (7)	C3—Fe1—C1	68.1 (3)
O1—C6—C5	116.8 (7)	C5—Fe1—C16	123.3 (3)
C12—C7—O1	127.3 (7)	C17—Fe1—C16	41.3 (4)
C12—C7—C8	125.3 (8)	C13—Fe1—C16	68.2 (3)
O1—C7—C8	107.4 (6)	C4—Fe1—C16	106.7 (3)
C7—C8—C9	119.1 (7)	C3—Fe1—C16	121.8 (3)
C7—C8—N1	109.5 (7)	C1—Fe1—C16	160.6 (3)
C9—C8—N1	131.4 (7)	C5—Fe1—C14	122.9 (3)
C10—C9—C8	116.0 (7)	C17—Fe1—C14	67.8 (3)
C10—C9—H9	122	C13—Fe1—C14	40.3 (3)
C8—C9—H9	122	C4—Fe1—C14	158.1 (3)
C9—C10—C11	124.4 (8)	C3—Fe1—C14	160.4 (3)
C9—C10—C11	118.5 (6)	C1—Fe1—C14	108.3 (3)
C11—C10—C11	117.1 (6)	C16—Fe1—C14	68.1 (3)
C10—C11—C12	119.7 (7)	C5—Fe1—C15	107.8 (3)
C10—C11—H11	120.2	C17—Fe1—C15	68.5 (4)
C12—C11—H11	120.2	C13—Fe1—C15	68.2 (3)
C7—C12—C11	115.6 (7)	C4—Fe1—C15	121.6 (3)
C7—C12—H12	122.2	C3—Fe1—C15	157.3 (3)
C11—C12—H12	122.2	C1—Fe1—C15	124.5 (3)
C17—C13—C14	108.9 (7)	C16—Fe1—C15	40.4 (3)
C17—C13—Fe1	70.0 (5)	C14—Fe1—C15	40.7 (3)
C14—C13—Fe1	70.2 (4)	C5—Fe1—C2	68.6 (3)
C17—C13—H13	125.6	C17—Fe1—C2	121.4 (4)
C14—C13—H13	125.6	C13—Fe1—C2	107.8 (3)
Fe1—C13—H13	125.8	C4—Fe1—C2	68.9 (3)

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C13—C14—C15	108.1 (7)	C3—Fe1—C2	40.7 (3)
C13—C14—Fe1	69.5 (4)	C1—Fe1—C2	40.3 (3)
C15—C14—Fe1	69.8 (4)	C16—Fe1—C2	157.6 (3)
C13—C14—H14	125.9	C14—Fe1—C2	124.1 (3)
C15—C14—H14	125.9	C15—Fe1—C2	160.7 (3)
Fe1—C14—H14	126.3	C6—N1—C8	103.5 (6)
C16—C15—C14	107.6 (8)	C7—O1—C6	103.9 (6)
C5—C1—C2—C3	0.0 (9)	C8—C9—C10—C11	0.0 (13)
Fe1—C1—C2—C3	58.7 (6)	C8—C9—C10—C11	179.5 (6)
C5—C1—C2—Fe1	-58.7 (6)	C9—C10—C11—C12	-0.3 (13)
C1—C2—C3—C4	-0.1 (9)	C11—C10—C11—C12	-179.9 (7)
Fe1—C2—C3—C4	58.9 (6)	O1—C7—C12—C11	179.6 (8)
C1—C2—C3—Fe1	-58.9 (6)	C8—C7—C12—C11	-1.0 (13)
C2—C3—C4—C5	0.1 (9)	C10—C11—C12—C7	0.8 (12)
Fe1—C3—C4—C5	59.4 (6)	C17—C13—C14—C15	-0.2 (10)
C2—C3—C4—Fe1	-59.3 (6)	Fe1—C13—C14—C15	59.3 (6)
C3—C4—C5—C1	-0.1 (9)	C17—C13—C14—Fe1	-59.5 (6)
Fe1—C4—C5—C1	59.7 (6)	C13—C14—C15—C16	0.3 (9)
C3—C4—C5—C6	-176.7 (8)	Fe1—C14—C15—C16	59.4 (6)
Fe1—C4—C5—C6	-116.9 (9)	C13—C14—C15—Fe1	-59.1 (6)
C3—C4—C5—Fe1	-59.8 (6)	C14—C15—C16—C17	-0.3 (9)
C2—C1—C5—C4	0.0 (9)	Fe1—C15—C16—C17	59.0 (6)
Fe1—C1—C5—C4	-59.7 (6)	C14—C15—C16—Fe1	-59.3 (6)
C2—C1—C5—C6	176.6 (8)	C14—C13—C17—C16	0.0 (10)
Fe1—C1—C5—C6	116.9 (9)	Fe1—C13—C17—C16	-59.7 (6)
C2—C1—C5—Fe1	59.7 (6)	C14—C13—C17—Fe1	59.6 (6)
C4—C5—C6—N1	-12.4 (14)	C15—C16—C17—C13	0.2 (9)
C1—C5—C6—N1	171.6 (8)	Fe1—C16—C17—C13	59.9 (6)
Fe1—C5—C6—N1	-100.2 (9)	C15—C16—C17—Fe1	-59.7 (6)
C4—C5—C6—O1	167.2 (8)	O1—C6—N1—C8	-1.3 (9)
C1—C5—C6—O1	-8.8 (12)	C5—C6—N1—C8	178.3 (8)
Fe1—C5—C6—O1	79.4 (9)	C7—C8—N1—C6	1.1 (9)
C12—C7—C8—C9	0.7 (12)	C9—C8—N1—C6	-179.7 (9)
O1—C7—C8—C9	-179.8 (7)	C12—C7—O1—C6	179.3 (8)
C12—C7—C8—N1	180.0 (8)	C8—C7—O1—C6	-0.2 (8)
O1—C7—C8—N1	-0.5 (8)	N1—C6—O1—C7	1.0 (9)
C7—C8—C9—C10	-0.1 (11)	C5—C6—O1—C7	-178.7 (7)
N1—C8—C9—C10	-179.2 (8)		

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