2-Amido-4-ferrocenythiazole

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The title compound, [Fe(C5H5)(C8H7N2S)], was synthesized by the direct reaction of acetylferrone, thiourea and resublimed iodine. The structure shows one molecule in the asymmetric unit. The aminothiazole ring makes an angle of 14.53 (13)° with the ferrocenyl ring to which it is attached. In the crystal, pairs of complex molecules interact via intermolecular N—H···C=N hydrogen bonds, forming a cyclic dimer which then interacts with other dimers through C—H···π interactions.

1. Chemical context

Recently, the synthesis of new hybrid compounds based on a ferrocenyl group linked to a five-membered heterocyclic unit has drawn attention (Sánchez-Rodríguez et al., 2017; Shao et al., 2006a). One important five-membered heterocycle is 2-aminothiazole, which is a versatile scaffold extensively used in various branches of chemistry including dyes and in the pharmaceutical industries. 2-Aminothiazole derivatives are widely used by medicinal chemists (Das et al., 2016) and have various applications in medicinal, agriculture and analytical chemistry. They are known to exhibit a wide variety of biological activities such as antiviral, antibacterial, antifungal, antitubercular, herbicidal and insecticidal (Mishra et al., 2017; Ji Ram et al., 2019; Dondoni, 2010). Thiazoles are also used as precursors or intermediates for the synthesis of a variety of heterocyclic compounds (Zeng et al., 2003). We report here the crystal and molecular structure of 2-amino-4-ferrocenylthiazole, which has not previously been reported.

2. Structural commentary

The title compound crystallizes in the monoclinic system, space group P2₁/c. The asymmetric unit contains one molecular unit as shown in Fig. 1. The C15—S11—C12 bond angle of 88.6 (2)° reflects the presence of a non-delocalized lone pair.
of electrons and is similar to that observed in other thiazoles. The length of the C12=N13 double bond is 1.306 (4) Å. The torsion angles in the amino substituted thiazole ring are: 1.1 (3)° for N13—C12—S11—C15 and 1.7 (4)° for N13—C14—C15—S11. All bond lengths and angles confirm the sp² hybridization for all C and N atoms.

The ferrocene moiety is in the staggered conformation. The influence of the steric hindrance caused by the organic groups is reflected in the torsion angle C5—C1—C14—C15, 17.0 (5)°, compared with the C2—C1—C14—N13 torsion angle of 13.2 (4)°. The steric effect is also evident in the dihedral angle of 14.77 (17)° subtended by the planes of the heterocycle (C14/C15/S11/C12/N13) and the Cp plane (C1–C5).

3. Supramolecular features

The structure is stabilized by intermolecular hydrogen bonding (N—H···N) and C—H···π interactions. For C10—H10···Cg(C1–C5) the H-to-ring distance is 2.89 Å, as shown in Table 1. As a result of intermolecular N—H···N interactions, a pseudo six-membered (N16/C12/N13/N16/C12/N13) ring is formed and this hydrogen bond, in addition to the C—H···π interaction, produces a packing into supramolecular layers parallel to the bc plane (Fig. 2). The structure presents very similar C=N distances and angles in the thiazole ring, as reported earlier for some similar compounds (Sánchez-Rodríguez et al., 2017; Shao et al., 2006b).

4. Database survey

A search of the Cambridge Structural Database (CSD, version 5.43, update of November 2021; Groom et al., 2016) for

**Table 1**

| Hydrogen-bond geometry (Å, °). |
|-----------------|---|---|---|---|
| D—H···A         | D—H | H···A | D···A | D···H |
| N16—H16A···N13  | 0.84 (2) | 2.14 (2) | 2.976 (4) | 173 (4) |
| C10—H10···Cg1   | 0.98 | 2.89 | 3.703 (3) | 141 |

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

**Table 2**

| Experimental details. |
|-----------------------|
| Crystal data          |
| Chemical formula      | [Fe(C₅H₅)(C₈H₇N₂S)] |
| M_r                   | 284.16 |
| Crystal system, space group | Monoclinic, P2₁/c |
| Temperature (K)       | 298 |
| a, b, c (Å)           | 14.4024 (4), 7.9621 (2), 10.3584 (3) |
| β (°)                 | 104.3453 (13) |
| V (Å³)                | 1150.80 (5) |
| Z                      | 4 |
| Radiation type        | Mo Kα |
| μ (mm⁻¹)              | 1.47 |
| Crystal size (mm)     | 0.27 × 0.16 × 0.14 |

**Data collection**

Diffractometer Bruker D8 Venture x-geometry
diffractometer 208039-01
Absorption correction Multi-scan (SADABS; Krause et al., 2015)

**Refinement**

R[F² > 2σ(F²)], wR(F²), S
0.050, 0.091, 1.02
3214
1
H-atoms treated by a mixture of independent and constrained refinement

**Computer programs:** APEX2 and SAINT (Bruker, 2014), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), XP (Siemens, 1998) and CIFTAB (Sheldrick, 2013).
4-ferrocenyl thiazoles gave eight hits. In six cases (GAVFIT, Yu et al., 2005; GAVFIT01, Yu et al., 2007; QAYSAL, Shao et al., 2006b; QAYSAL01, Shao et al., 2006a; RAPQAB, Shao et al., 2005; RAPQAB01, Shao et al., 2006a), the thiazole ring is substituted. In two cases there is no substitution in the thiazole ring (GUPKAG, Xu et al., 2020 and PAWWEQ, Plazuk et al., 2005) with PAWWEQ being a diferrocenyl compound. In all eight cases, the bond lengths and angles confirm the sp² hybridization for all C and N atoms.

5. Synthesis and crystallization
The title compound was synthesized according to the reported method (Chopra et al., 2015). The crude product was purified by column chromatography over silica and suitable crystals were obtained after recrystallization of the solid from a 1:1 hexane-dichloromethane mixture by slow evaporation. The compound 2-amino-4-ferrocenylthiazole was further characterized by ¹H NMR and IR–ATR. FT–IR (ATR, cm⁻¹) ν 3099 (ArCH), 2921 (CH₃), 1658 (C=N); ¹HNMR (300 MHz, CDCl₃): 4.62 (2H, t, subst. Cp); 4.25 (2H, t, subst. Cp); 4.10 (5H, s, subst. Cp); 5.00 (2H, –NH₂), 6.35 (1H, C—H).

6. Refinement details
Crystal data, data collection and structure refinement details are summarized in Table 2. N-bound H atoms were refined isotropically with \(U_{eq}(H) = 1.2U_{eq}(N)\). C-bound H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and refined with isotropically \(U_{eq}(H) = 1.2U_{eq}(C)\) using a riding model.

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2-Amino-4-ferrocenylthiazole

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Computing details

Data collection: APEX2 (Bruker, 2014); cell refinement: APEX2 (Bruker, 2014); data reduction: SAINT (Bruker, 2014); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: SHELXL (Sheldrick, 2015b); molecular graphics: XP (Siemens, 1998); software used to prepare material for publication: CIFTAB (Sheldrick, 2013).

2-Amino-4-ferrocenylthiazole

Crystal data

\[\text{[Fe(C}_5\text{H}_5\text{)(C}_8\text{H}_7\text{N}_2\text{S})]\]

\[M_r = 284.16\]

Monoclinic, \(P2_1/c\)

\(a = 14.4024 (4) \text{ Å}\)

\(b = 7.9621 (2) \text{ Å}\)

\(c = 10.3584 (3) \text{ Å}\)

\(β = 104.3453 (13)°\)

\(V = 1150.80 (5) \text{ Å}^3\)

\(Z = 4\)

\(F(000) = 584\)

\(D_x = 1.640 \text{ Mg m}^{-3}\)

\(\text{Mo } K\alpha \text{ radiation, } λ = 0.71073 \text{ Å}\)

Cell parameters from 5893 reflections

\(θ = 2.9 – 30.0°\)

\(µ = 1.47 \text{ mm}^{-1}\)

\(T = 298 \text{ K}\)

Prism, orange

\(0.27 \times 0.16 \times 0.14 \text{ mm}\)

Data collection

Bruker D8 Venture \(κ\)-geometry
diffractometer 208039-01

Radiation source: micro-focus X-ray source

Helios multilayer mirror monochromator

Detector resolution: 52.0833 pixels mm\(^{-1}\)

\(φ \text{ and } ω\)–scans

Absorption correction: multi-scan

(SADABS; Krause et al., 2015)

\(T_{\text{min}} = 0.656, T_{\text{max}} = 0.746\)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R[F^2 > 2σ(F^2)] = 0.050\)

\(wR(F^2) = 0.091\)

\(S = 1.02\)

3214 reflections

160 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: mixed

\(H\) atoms treated by a mixture of independent and constrained refinement

\(w = 1/[σ(Fo^2) + (0.024P)^2 + 0.7338P]\)

where \(P = (Fo^2 + 2Fc^2)/3\)

\((Δ/σ)_{\text{max}} < 0.001\)

\(Δρ_{\text{max}} = 0.44 \text{ e Å}^{-3}\)

\(Δρ_{\text{min}} = -0.43 \text{ e Å}^{-3}\)
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 (Å²)**

| Atom | x       | y       | z       | Uiso*       |
|------|---------|---------|---------|-------------|
| Fe1  | 0.17036 (3) | 0.50999 (5) | 0.21675 (4) | 0.02688 (13) |
| C1   | 0.2361 (2)  | 0.7055 (3)  | 0.3316 (3)  | 0.0293 (7)   |
| C2   | 0.2072 (2)  | 0.5816 (4)  | 0.4119 (3)  | 0.0347 (7)   |
| H2   | 0.249851    | 0.519784    | 0.484765    | 0.042*       |
| C3   | 0.1066 (2)  | 0.5605 (4)  | 0.3683 (3)  | 0.0378 (8)   |
| H3   | 0.067801    | 0.482058    | 0.405807    | 0.045*       |
| C5   | 0.1513 (2)  | 0.7608 (4)  | 0.2371 (3)  | 0.0354 (8)   |
| H5   | 0.148594    | 0.845906    | 0.167931    | 0.043*       |
| C4   | 0.0721 (2)  | 0.6712 (4)  | 0.2603 (3)  | 0.0390 (8)   |
| H4   | 0.005144    | 0.683301    | 0.210031    | 0.047*       |
| C6   | 0.2513 (2)  | 0.4562 (4)  | 0.0875 (3)  | 0.0390 (8)   |
| H6   | 0.301224    | 0.528302    | 0.067788    | 0.047*       |
| C7   | 0.2651 (2)  | 0.3335 (4)  | 0.1884 (3)  | 0.0401 (8)   |
| H7   | 0.326028    | 0.304522    | 0.250824    | 0.048*       |
| C8   | 0.1747 (2)  | 0.2590 (4)  | 0.1828 (3)  | 0.0436 (9)   |
| H8   | 0.162060    | 0.169787    | 0.241401    | 0.052*       |
| C9   | 0.1063 (2)  | 0.3352 (4)  | 0.0782 (3)  | 0.0417 (8)   |
| H9   | 0.037655    | 0.309044    | 0.051734    | 0.050*       |
| C10  | 0.1538 (2)  | 0.4568 (4)  | 0.0194 (3)  | 0.0388 (8)   |
| H10  | 0.123912    | 0.530116    | −0.055375   | 0.047*       |
| S11  | 0.48146 (6) | 0.92268 (11)| 0.31997 (10)| 0.0468 (3)   |
| C12  | 0.4914 (2)  | 0.7406 (4)  | 0.4136 (3)  | 0.0340 (7)   |
| N13  | 0.41026 (17)| 0.6692 (3)  | 0.4162 (3)  | 0.0313 (6)   |
| C14  | 0.3340 (2)  | 0.7625 (4)  | 0.3407 (3)  | 0.0301 (7)   |
| C15  | 0.3588 (2)  | 0.9019 (4)  | 0.2849 (3)  | 0.0407 (8)   |
| H15  | 0.315506    | 0.977392    | 0.234051    | 0.049*       |
| N16  | 0.5779 (2)  | 0.6798 (4)  | 0.4780 (4)  | 0.0506 (9)   |
| H16A | 0.580 (2)   | 0.585 (3)   | 0.514 (3)   | 0.061*       |
| H16B | 0.627 (2)   | 0.732 (4)   | 0.469 (4)   | 0.061*       |

**Atomic displacement parameters (Å²)**

|   | U11  | U22  | U33  | U12  | U13  | U23  |
|---|------|------|------|------|------|------|
| Fe1 | 0.0253 (2) | 0.0294 (2) | 0.0264 (2) | 0.00356 (18) | 0.00735 (17) | −0.0012 (2) |
| C1  | 0.0303 (17) | 0.0283 (16) | 0.0294 (18) | 0.0051 (12) | 0.0075 (14) | −0.0029 (13) |
| C2  | 0.0349 (18) | 0.0426 (18) | 0.0263 (18) | 0.0062 (14) | 0.0071 (14) | −0.0018 (15) |
| C3  | 0.0341 (18) | 0.050 (2) | 0.035 (2) | 0.0000 (15) | 0.0180 (15) | −0.0075 (16) |
| C5  | 0.0387 (19) | 0.0287 (16) | 0.036 (2) | 0.0100 (14) | 0.0042 (16) | −0.0040 (14) |
| C4  | 0.0283 (18) | 0.048 (2) | 0.039 (2) | 0.0094 (15) | 0.0060 (15) | −0.0144 (17) |
### Geometric parameters (Å, °)

| Bond/Angle                      | Distance/Angle | Distance/Angle |
|---------------------------------|----------------|----------------|
| Fe1—C6                          | 2.027 (3)       | C6—C10 1.408 (4) |
| Fe1—C7                          | 2.030 (3)       | C6—C7 1.408 (4) |
| Fe1—C8                          | 2.033 (3)       | C6—H6 0.980 |
| Fe1—C5                          | 2.034 (3)       | C7—C8 1.419 (4) |
| Fe1—C2                          | 2.040 (3)       | C7—H7 0.980 |
| Fe1—C4                          | 2.043 (3)       | C7—C9 1.408 (4) |
| Fe1—C10                         | 2.043 (3)       | C8—C9 1.408 (4) |
| Fe1—C3                          | 2.045 (3)       | C8—H8 0.980 |
| Fe1—C9                          | 2.047 (3)       | C9—C10 1.409 (4) |
| C1—C2                           | 1.417 (4)       | C9—H9 0.980 |
| C1—C5                           | 1.432 (4)       | C9—H9 0.980 |
| C1—C14                          | 1.462 (4)       | C10—H10 1.721 (3) |
| C2—C3                           | 1.417 (4)       | S11—C15 1.721 (3) |
| C3—C4                           | 1.417 (4)       | S11—C12 1.730 (3) |
| C3—H3                           | 0.9800          | C12—N13 1.306 (4) |
| C5—C4                           | 1.416 (4)       | C12—N16 1.349 (4) |
| C5—H5                           | 0.9800          | C13—C14 1.394 (3) |
| C6—Fe1—C7                      | 40.61 (12)      | C14—C15 1.340 (4) |
| C6—Fe1—C8                      | 68.33 (13)      | C15—H15 0.9300 |
| C7—Fe1—C8                      | 40.88 (12)      | N16—H16A 0.84 (2) |
| C6—Fe1—C9                      | 112.99 (13)     | N16—H16B 0.84 (2) |
| C7—Fe1—C5                      | 143.86 (14)     | C4—C3—H3 126.0 |
| C8—Fe1—C5                      | 173.68 (13)     | C2—C3—H3 126.0 |
| C6—Fe1—C5                      | 112.99 (13)     | C4—C5—H3 126.0 |
| C7—Fe1—C5                      | 143.86 (14)     | C4—C5—Fe1 108.4 (3) |
| C8—Fe1—C5                      | 173.68 (13)     | C1—C5—Fe1 70.02 (17) |
| C6—Fe1—C2                      | 131.49 (13)     | C1—C5—H5 125.8 |
| C7—Fe1—C2                      | 108.54 (13)     | C4—C5—H5 125.8 |
| C8—Fe1—C2                      | 115.77 (13)     | C5—C4—H5 125.8 |
| C5—Fe1—C7                      | 68.37 (13)      | C3—C4—C5 107.9 (3) |
| C6—Fe1—C4                      | 145.32 (14)     | C3—C4—Fe1 69.85 (17) |
| C7—Fe1—C4                      | 173.96 (14)     | C5—C4—Fe1 69.34 (17) |
| C8—Fe1—C4                      | 135.13 (14)     | C3—C4—H4 126.0 |

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| Bond                  | Distance (Å) | Bond                  | Distance (Å) |
|----------------------|--------------|----------------------|--------------|
| C5—Fe1—C4           | 40.64 (12)   | C5—C4—H4            | 126.0        |
| C2—Fe1—C4           | 68.26 (12)   | Fe1—C4—H4           | 126.0        |
| C6—Fe1—C1           | 106.63 (13)  | C10—C6—C7           | 108.3 (3)    |
| C7—Fe1—C1           | 112.38 (13)  | C10—C6—Fe1          | 70.40 (18)   |
| C8—Fe1—C1           | 145.08 (13)  | C7—C6—Fe1           | 69.82 (18)   |
| C5—Fe1—C3           | 41.12 (11)   | C10—C6—H6           | 125.9        |
| C2—Fe1—C1           | 40.62 (12)   | C7—C6—H6            | 125.9        |
| C4—Fe1—C1           | 68.84 (12)   | Fe1—C6—H6           | 125.9        |
| C6—Fe1—C10          | 40.46 (12)   | C6—C7—C8            | 107.5 (3)    |
| C7—Fe1—C10          | 68.14 (13)   | C6—C7—Fe1           | 69.56 (17)   |
| C8—Fe1—C10          | 67.91 (13)   | C8—C7—Fe1           | 69.66 (18)   |
| C5—Fe1—C10          | 108.79 (13)  | C6—C7—H7            | 126.2        |
| C2—Fe1—C10          | 170.67 (13)  | C8—C7—H7            | 126.2        |
| C4—Fe1—C10          | 115.84 (13)  | Fe1—C7—H7           | 126.2        |
| C1—Fe1—C10          | 131.53 (13)  | C9—C8—C7            | 108.1 (3)    |
| C6—Fe1—C3           | 171.70 (13)  | C9—C8—Fe1           | 70.36 (18)   |
| C7—Fe1—C3           | 133.85 (14)  | C7—C8—Fe1           | 69.46 (18)   |
| C8—Fe1—C3           | 111.39 (13)  | C9—C8—H8            | 125.9        |
| C5—Fe1—C3           | 68.26 (13)   | C7—C8—H8            | 125.9        |
| C2—Fe1—C3           | 40.58 (12)   | Fe1—C8—H8           | 125.9        |
| C4—Fe1—C3           | 40.48 (13)   | C8—C9—C10           | 107.9 (3)    |
| C1—Fe1—C3           | 68.58 (13)   | C8—C9—Fe1           | 69.26 (18)   |
| C10—Fe1—C3          | 147.70 (13)  | C10—C9—Fe1          | 69.70 (18)   |
| C6—Fe1—C9           | 68.10 (13)   | C8—C9—H9            | 126.1        |
| C7—Fe1—C9           | 68.31 (13)   | C10—C9—H9           | 126.1        |
| C8—Fe1—C9           | 40.38 (12)   | Fe1—C9—H9           | 126.1        |
| C5—Fe1—C9           | 133.72 (13)  | C6—C10—C9           | 108.2 (3)    |
| C2—Fe1—C9           | 147.76 (14)  | C6—C10—Fe1          | 69.14 (18)   |
| C4—Fe1—C9           | 111.42 (13)  | C9—C10—Fe1          | 70.01 (18)   |
| C1—Fe1—C9           | 171.57 (13)  | C6—C10—H10          | 125.9        |
| C10—Fe1—C9          | 40.29 (13)   | C9—C10—H10          | 125.9        |
| C3—Fe1—C9           | 117.46 (14)  | Fe1—C10—H10         | 125.9        |
| C2—C1—C5            | 106.9 (3)    | C15—S11—C12         | 88.62 (15)   |
| C2—C1—C14           | 126.6 (3)    | N13—C12—N16         | 123.7 (3)    |
| C5—C1—C14           | 126.4 (3)    | N13—C12—S11         | 115.2 (2)    |
| C2—C1—Fe1           | 69.56 (17)   | N16—C12—S11         | 121.1 (2)    |
| C5—C1—Fe1           | 69.09 (16)   | C12—N13—C14         | 110.0 (3)    |
| C14—C1—Fe1          | 125.0 (2)    | C15—C14—N13         | 115.2 (3)    |
| C3—C2—C1            | 108.7 (3)    | C15—C14—C1          | 125.8 (3)    |
| C3—C2—Fe1           | 69.93 (17)   | N13—C14—C1          | 119.0 (3)    |
| C1—C2—Fe1           | 69.82 (17)   | C14—C15—S11         | 111.0 (2)    |
| C3—C2—H2            | 125.6        | C14—C15—H15         | 124.5        |
| C1—C2—H2            | 125.6        | S11—C15—H15         | 124.5        |
| Fe1—C2—H2           | 125.6        | C12—N16—H16A        | 118 (2)      |
| C4—C3—C2            | 108.0 (3)    | C12—N16—H16B        | 118 (2)      |
| C4—C3—Fe1           | 69.67 (18)   | H16A—N16—H16B       | 123 (3)      |
| C2—C3—Fe1           | 69.49 (17)   |                       |              |
C5—C1—C2—C3  0.0 (3)  C7—C8—C9—C10  −0.2 (4)
C14—C1—C2—C3  −178.4 (3)  Fe1—C8—C9—C10  59.2 (2)
Fe1—C1—C2—C3  −59.3 (2)  C7—C8—C9—Fe1  −59.4 (2)
C5—C1—C2—Fe1  59.2 (2)  C7—C6—C10—C9  0.5 (3)
C14—C1—C2—Fe1  −119.1 (3)  Fe1—C6—C10—C9  −59.3 (2)
C1—C2—C3—C4  0.0 (3)  C7—C6—C10—Fe1  59.8 (2)
Fe1—C2—C3—C4  −59.2 (2)  C8—C9—C10—C6  −0.2 (4)
C1—C2—C3—Fe1  59.2 (2)  Fe1—C9—C10—C6  58.8 (2)
C2—C1—C5—C4  0.0 (3)  C8—C9—C10—Fe1  −58.9 (2)
C14—C1—C5—C4  178.4 (3)  C15—S11—C12—N13  1.1 (3)
Fe1—C1—C5—C4  59.6 (2)  C15—S11—C12—N16  −179.0 (3)
C2—C1—C5—Fe1  −59.5 (2)  N16—C12—N13—C14  179.7 (3)
C14—C1—C5—Fe1  118.8 (3)  S11—C12—N13—C14  −0.4 (3)
C2—C3—C4—C5  0.0 (3)  C12—N13—C14—C15  −0.9 (4)
Fe1—C3—C4—C5  −59.1 (2)  C12—N13—C14—C1  −179.3 (3)
C2—C3—C4—Fe1  59.1 (2)  C2—C1—C14—C15  −165.0 (3)
C1—C5—C4—C3  0.0 (3)  C5—C1—C14—C15  17.0 (5)
Fe1—C5—C4—C3  59.4 (2)  Fe1—C1—C14—C15  105.6 (3)
C1—C5—C4—Fe1  −59.4 (2)  C2—C1—C14—N13  13.2 (4)
C10—C6—C7—C8  −0.6 (3)  C5—C1—C14—N13  −164.9 (3)
Fe1—C6—C7—C8  59.6 (2)  Fe1—C1—C14—N13  −76.2 (3)
C10—C6—C7—Fe1  −60.1 (2)  N13—C14—C15—S11  1.7 (4)
C6—C7—C8—C9  0.5 (4)  C1—C14—C15—S11  180.0 (2)
Fe1—C7—C8—C9  60.0 (2)  C12—S11—C15—C14  −1.6 (3)
C6—C7—C8—Fe1  −59.5 (2)

_Hydrogen-bond geometry (Å, °)_

_Cg1 is the centroid of the C1–C5 Cp ring._

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| N16—H16···N131 | 0.84 (2) | 2.14 (2) | 2.976 (4) | 173 (4) |
| C10—H10···Cg111 | 0.98 | 2.89 | 3.703 (3) | 141 |

Symmetry codes: (i) −x+1, −y+1, −z+1; (ii) x, −y+3/2, z−1/2.