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# Crystal structure of cyclic tris(ferrocene-1,1′-diyl)

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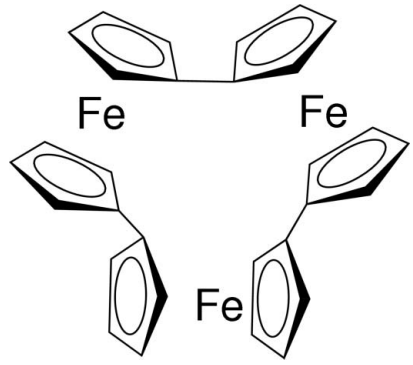
The molecular structure of the trinuclear title compound, $[Fe_3(C_{10}H_8)_3]$ {systematic name: tris[$\mu$-($\eta^5$:$\eta^5$)-1,1′-bicyclopentadienyl]triiron(II)}, consists of three ferrocene subunits (each with an eclipsed conformation) that are condensed *via* C—C bonds of the fulvalene moieties into a cyclic trimer. The angles between the planes of the cyclopentadienyl (Cp) rings within the three fulvalene moieties are 76.1 (3), 80.9 (3) and 81.7 (3)°. In the crystal, C—H$\cdots\pi$ interactions between neighbouring molecules lead to the cohesion of the structure.

**Keywords:** crystal structure; ferrocene; eclipsed conformation; C—H$\cdots\pi$ interactions.

**CCDC reference**: 1016442

## 1. Related literature

The title compound was obtained as a side product during the synthesis of (ferrocene-1,1′-diyl)bis(*H*-phosphinic acids) (Shekurov *et al.*, 2014). In the molecular structure of the related binuclear ferrocene derivative bis(fulvalene)diiron (Churchill & Wormald, 1969), the Cp rings of the fulvalene moieties are coplanar.




## 2. Experimental

### 2.1. Crystal data

$[Fe_3(C_{10}H_8)_3]$
$M_r$ = 552.04
Triclinic, $P\overline{1}$
$a$ = 9.9006 (16) Å
$b$ = 10.5544 (17) Å
$c$ = 12.448 (3) Å
$\alpha$ = 109.197 (5)°
$\beta$ = 100.205 (5)°
$\gamma$ = 108.940 (3)°
$V$ = 1101.7 (4) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.97 mm$^{-1}$
$T$ = 296 K
0.30 × 0.25 × 0.20 mm

### 2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.590, $T_{max}$ = 0.695
14158 measured reflections
4270 independent reflections
2958 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.070

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.076
$S$ = 1.31
4270 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.65 e Å$^{-3}$

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

*Cg*1 and *Cg*4 are the centroids of the C1–C5 and C16–C20 rings, respectively.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C30—H30$\cdots$*Cg*1$^{i}$ | 0.98 | 2.89 | 3.668 (5) | 137 |
| C28—H28$\cdots$*Cg*4$^{ii}$ | 0.98 | 2.70 | 3.601 (6) | 153 |

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: WM5035).

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# supporting information

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## Crystal structure of cyclic tris(ferrocene-1,1′-diyl)

**Ruslan Shekurov, Vasili Miluykov, Olga Kataeva, Artem Tufatullin and Oleg Sinyashin**

### S1. Experimental

The title compound, $[1,1'\text{-Fc}]_3$ (Fc = ferrocene), was obtained as a side product during the synthesis of (ferrocene-1,1′-diyl)bis(*H*-phosphonic acids) (Shekurov *et al.*, 2014) by reaction of 1,1′-dilithiumferrocene, $Li_2Fc$, with bis(diethylamino)chlorophosphite $(NEt_2)_2ClP$ in hexane. Orange crystals of the title compound were obtained on standing of solutions of $1,1'\text{-Fc}(P(NEt_2)_2)_2$ in hexane.

### S2. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.98 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

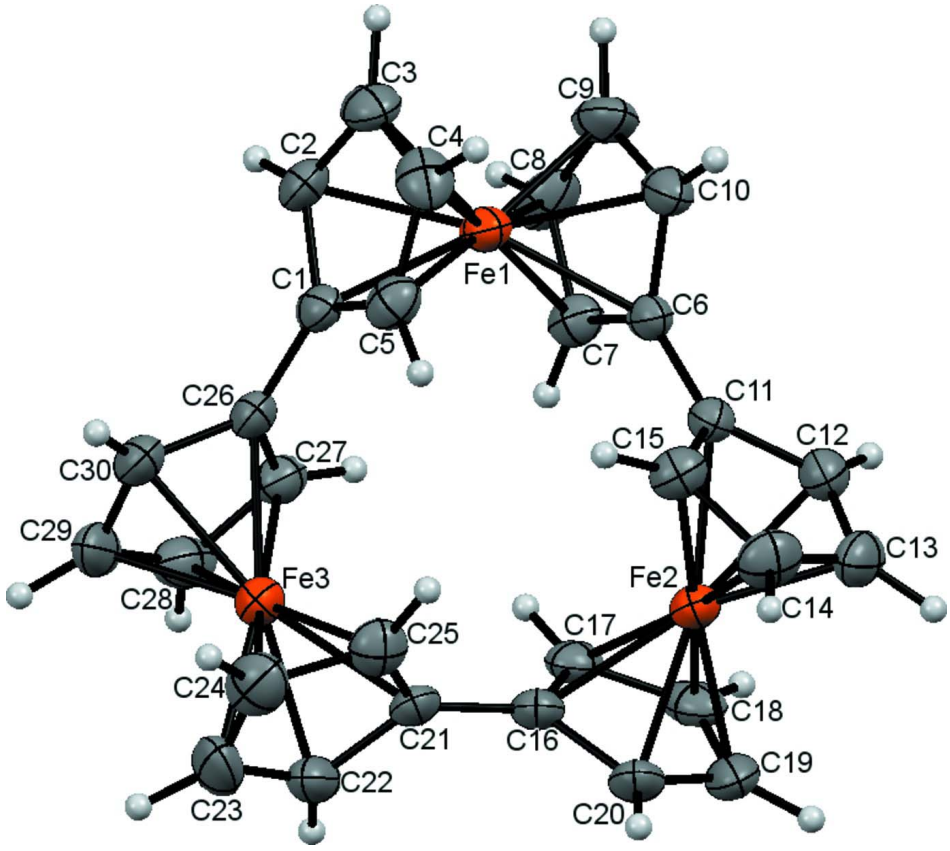


**Figure 1**

The molecular structure of the title compound, with displacement ellipsoids displayed at the 50% probability level.

**Tris[$\mu$-($\eta^5$:$\eta^5$)-1,1′-bicyclopentadienyl]triiron(II)**

*Crystal data*

$[Fe_3(C_{10}H_8)_3]$
$M_r = 552.04$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.9006$ (16) Å
$b = 10.5544$ (17) Å
$c = 12.448$ (3) Å
$\alpha = 109.197$ (5)°
$\beta = 100.205$ (5)°
$\gamma = 108.940$ (3)°
$V = 1101.7$ (4) Å$^3$
$Z = 2$
$F(000) = 564$
$D_x = 1.664$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3519 reflections
$\theta = 2.2$–$28.4°$
$\mu = 1.97$ mm$^{-1}$
$T = 296$ K
Prism, orange
0.30 × 0.25 × 0.20 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.590$, $T_{max} = 0.695$
14158 measured reflections
4270 independent reflections
2958 reflections with $I > 2\sigma(I)$
$R_{int} = 0.070$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.8°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.076$
$S = 1.31$
4270 reflections
298 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
$w = 1/[\sigma^2(F_o^2) + (0.P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.65$ e Å$^{-3}$
$\Delta\rho_{min} = -0.65$ 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.6533 (4) | 0.5589 (4) | 0.3621 (4) | 0.0316 (10) |
| C2 | 0.6144 (5) | 0.6798 (4) | 0.3643 (4) | 0.0385 (11) |
| H2 | 0.5183 | 0.6725 | 0.3192 | 0.046* |

| | | | | |
|---|---|---|---|---|
| C3 | 0.7420 (5) | 0.8118 (4) | 0.4438 (4) | 0.0438 (12) |
| H3 | 0.7486 | 0.9119 | 0.4633 | 0.053* |
| C4 | 0.8562 (5) | 0.7750 (4) | 0.4912 (4) | 0.0443 (12) |
| H4 | 0.9559 | 0.8446 | 0.5488 | 0.053* |
| C5 | 0.8019 (5) | 0.6200 (4) | 0.4408 (4) | 0.0371 (11) |
| H5 | 0.8589 | 0.5639 | 0.4565 | 0.044* |
| C6 | 0.9417 (4) | 0.6495 (4) | 0.2144 (4) | 0.0308 (10) |
| C7 | 0.7931 (4) | 0.5911 (4) | 0.1360 (4) | 0.0349 (10) |
| H7 | 0.7313 | 0.4869 | 0.0834 | 0.042* |
| C8 | 0.7472 (5) | 0.7075 (5) | 0.1485 (4) | 0.0461 (12) |
| H8 | 0.6496 | 0.6985 | 0.1046 | 0.055* |
| C9 | 0.8672 (6) | 0.8386 (5) | 0.2338 (5) | 0.0521 (14) |
| H9 | 0.8680 | 0.9372 | 0.2596 | 0.062* |
| C10 | 0.9859 (5) | 0.8044 (4) | 0.2741 (4) | 0.0417 (12) |
| H10 | 1.0835 | 0.8752 | 0.3344 | 0.050* |
| C11 | 1.0423 (4) | 0.5741 (4) | 0.2255 (4) | 0.0302 (10) |
| C12 | 1.1292 (4) | 0.5442 (4) | 0.1481 (4) | 0.0360 (11) |
| H12 | 1.1255 | 0.5618 | 0.0753 | 0.043* |
| C13 | 1.2229 (4) | 0.4864 (4) | 0.1958 (4) | 0.0435 (12) |
| H13 | 1.2957 | 0.4572 | 0.1617 | 0.052* |
| C14 | 1.1941 (5) | 0.4781 (4) | 0.2998 (4) | 0.0459 (12) |
| H14 | 1.2430 | 0.4419 | 0.3512 | 0.055* |
| C15 | 1.0833 (4) | 0.5324 (4) | 0.3187 (4) | 0.0366 (11) |
| H15 | 1.0408 | 0.5384 | 0.3846 | 0.044* |
| C16 | 0.8243 (4) | 0.1780 (4) | 0.1464 (4) | 0.0323 (10) |
| C17 | 0.7861 (4) | 0.2140 (4) | 0.0490 (4) | 0.0362 (11) |
| H17 | 0.7038 | 0.2437 | 0.0309 | 0.043* |
| C18 | 0.8882 (5) | 0.2040 (4) | −0.0165 (4) | 0.0429 (12) |
| H18 | 0.8874 | 0.2229 | −0.0885 | 0.051* |
| C19 | 0.9902 (5) | 0.1617 (4) | 0.0398 (4) | 0.0465 (12) |
| H19 | 1.0729 | 0.1449 | 0.0134 | 0.056* |
| C20 | 0.9525 (4) | 0.1453 (4) | 0.1404 (4) | 0.0409 (12) |
| H20 | 1.0047 | 0.1157 | 0.1958 | 0.049* |
| C21 | 0.7380 (4) | 0.1526 (4) | 0.2280 (4) | 0.0318 (10) |
| C22 | 0.6042 (4) | 0.0233 (4) | 0.1953 (5) | 0.0440 (12) |
| H22 | 0.5492 | −0.0544 | 0.1141 | 0.053* |
| C23 | 0.5647 (5) | 0.0263 (5) | 0.2986 (5) | 0.0543 (14) |
| H23 | 0.4787 | −0.0492 | 0.3023 | 0.065* |
| C24 | 0.6711 (5) | 0.1558 (5) | 0.3958 (5) | 0.0511 (13) |
| H24 | 0.6718 | 0.1867 | 0.4793 | 0.061* |
| C25 | 0.7783 (5) | 0.2333 (4) | 0.3531 (4) | 0.0391 (11) |
| H25 | 0.8646 | 0.3280 | 0.4018 | 0.047* |
| C26 | 0.5445 (4) | 0.4019 (4) | 0.2984 (4) | 0.0325 (10) |
| C27 | 0.4946 (4) | 0.3110 (4) | 0.1753 (4) | 0.0374 (11) |
| H27 | 0.5360 | 0.3358 | 0.1153 | 0.045* |
| C28 | 0.3759 (5) | 0.1773 (4) | 0.1525 (5) | 0.0478 (12) |
| H28 | 0.3196 | 0.0944 | 0.0739 | 0.057* |
| C29 | 0.3508 (5) | 0.1844 (5) | 0.2608 (5) | 0.0498 (13) |

| | | | | |
|---|---|---|---|---|
| H29 | 0.2741 | 0.1073 | 0.2714 | 0.060* |
| C30 | 0.4563 (5) | 0.3216 (4) | 0.3530 (4) | 0.0414 (11) |
| H30 | 0.4651 | 0.3567 | 0.4383 | 0.050* |
| Fe1 | 0.79971 (6) | 0.69662 (6) | 0.30904 (5) | 0.03287 (17) |
| Fe2 | 1.00395 (6) | 0.35453 (6) | 0.15645 (5) | 0.03206 (17) |
| Fe3 | 0.56465 (6) | 0.20506 (6) | 0.27057 (6) | 0.03564 (18) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.038 (3) | 0.031 (2) | 0.032 (3) | 0.018 (2) | 0.019 (2) | 0.013 (2) |
| C2 | 0.038 (3) | 0.040 (2) | 0.047 (3) | 0.024 (2) | 0.023 (2) | 0.017 (2) |
| C3 | 0.056 (3) | 0.032 (2) | 0.043 (3) | 0.021 (2) | 0.023 (3) | 0.009 (2) |
| C4 | 0.042 (3) | 0.044 (3) | 0.030 (3) | 0.008 (2) | 0.008 (2) | 0.007 (2) |
| C5 | 0.042 (3) | 0.043 (3) | 0.032 (3) | 0.023 (2) | 0.014 (2) | 0.016 (2) |
| C6 | 0.039 (3) | 0.028 (2) | 0.034 (3) | 0.016 (2) | 0.020 (2) | 0.016 (2) |
| C7 | 0.043 (3) | 0.038 (2) | 0.031 (3) | 0.021 (2) | 0.014 (2) | 0.016 (2) |
| C8 | 0.055 (3) | 0.066 (3) | 0.044 (3) | 0.043 (3) | 0.020 (3) | 0.034 (3) |
| C9 | 0.077 (4) | 0.040 (3) | 0.067 (4) | 0.037 (3) | 0.039 (3) | 0.034 (3) |
| C10 | 0.051 (3) | 0.029 (2) | 0.047 (3) | 0.014 (2) | 0.027 (3) | 0.014 (2) |
| C11 | 0.032 (2) | 0.025 (2) | 0.034 (3) | 0.0104 (19) | 0.014 (2) | 0.011 (2) |
| C12 | 0.036 (3) | 0.033 (2) | 0.041 (3) | 0.012 (2) | 0.016 (2) | 0.015 (2) |
| C13 | 0.028 (3) | 0.040 (3) | 0.058 (4) | 0.015 (2) | 0.014 (3) | 0.015 (3) |
| C14 | 0.042 (3) | 0.051 (3) | 0.048 (3) | 0.026 (2) | 0.007 (3) | 0.021 (3) |
| C15 | 0.040 (3) | 0.038 (2) | 0.034 (3) | 0.020 (2) | 0.011 (2) | 0.013 (2) |
| C16 | 0.037 (3) | 0.024 (2) | 0.040 (3) | 0.016 (2) | 0.014 (2) | 0.014 (2) |
| C17 | 0.039 (3) | 0.022 (2) | 0.041 (3) | 0.012 (2) | 0.009 (2) | 0.007 (2) |
| C18 | 0.065 (3) | 0.025 (2) | 0.035 (3) | 0.016 (2) | 0.019 (3) | 0.008 (2) |
| C19 | 0.056 (3) | 0.031 (2) | 0.060 (4) | 0.022 (2) | 0.035 (3) | 0.015 (2) |
| C20 | 0.044 (3) | 0.031 (2) | 0.061 (4) | 0.023 (2) | 0.023 (3) | 0.025 (2) |
| C21 | 0.033 (2) | 0.029 (2) | 0.041 (3) | 0.020 (2) | 0.015 (2) | 0.016 (2) |
| C22 | 0.038 (3) | 0.029 (2) | 0.067 (4) | 0.016 (2) | 0.020 (3) | 0.018 (2) |
| C23 | 0.052 (3) | 0.052 (3) | 0.088 (5) | 0.026 (3) | 0.041 (3) | 0.048 (3) |
| C24 | 0.064 (3) | 0.061 (3) | 0.052 (4) | 0.035 (3) | 0.028 (3) | 0.036 (3) |
| C25 | 0.036 (3) | 0.045 (3) | 0.039 (3) | 0.020 (2) | 0.007 (2) | 0.020 (2) |
| C26 | 0.032 (2) | 0.034 (2) | 0.039 (3) | 0.019 (2) | 0.018 (2) | 0.016 (2) |
| C27 | 0.037 (3) | 0.034 (2) | 0.040 (3) | 0.018 (2) | 0.013 (2) | 0.012 (2) |
| C28 | 0.037 (3) | 0.035 (3) | 0.061 (4) | 0.016 (2) | 0.005 (3) | 0.011 (3) |
| C29 | 0.028 (3) | 0.038 (3) | 0.087 (4) | 0.015 (2) | 0.024 (3) | 0.026 (3) |
| C30 | 0.046 (3) | 0.041 (3) | 0.053 (3) | 0.027 (2) | 0.029 (3) | 0.022 (3) |
| Fe1 | 0.0387 (4) | 0.0287 (3) | 0.0351 (4) | 0.0173 (3) | 0.0150 (3) | 0.0128 (3) |
| Fe2 | 0.0331 (4) | 0.0287 (3) | 0.0385 (4) | 0.0164 (3) | 0.0138 (3) | 0.0139 (3) |
| Fe3 | 0.0332 (4) | 0.0325 (3) | 0.0452 (5) | 0.0159 (3) | 0.0166 (3) | 0.0163 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C5 | 1.414 (5) | C16—C17 | 1.411 (5) |
| C1—C2 | 1.442 (5) | C16—C20 | 1.427 (5) |

| | | | |
|---|---|---|---|
| C1—C26 | 1.487 (5) | C16—C21 | 1.474 (5) |
| C1—Fe1 | 2.062 (4) | C16—Fe2 | 2.066 (4) |
| C2—C3 | 1.422 (5) | C17—C18 | 1.415 (5) |
| C2—Fe1 | 2.046 (4) | C17—Fe2 | 2.058 (4) |
| C2—H2 | 0.9800 | C17—H17 | 0.9800 |
| C3—C4 | 1.407 (5) | C18—C19 | 1.400 (5) |
| C3—Fe1 | 2.017 (4) | C18—Fe2 | 2.042 (4) |
| C3—H3 | 0.9800 | C18—H18 | 0.9800 |
| C4—C5 | 1.412 (5) | C19—C20 | 1.415 (5) |
| C4—Fe1 | 2.039 (4) | C19—Fe2 | 2.019 (4) |
| C4—H4 | 0.9800 | C19—H19 | 0.9800 |
| C5—Fe1 | 2.054 (4) | C20—Fe2 | 2.030 (4) |
| C5—H5 | 0.9800 | C20—H20 | 0.9800 |
| C6—C7 | 1.415 (5) | C21—C25 | 1.413 (5) |
| C6—C10 | 1.427 (5) | C21—C22 | 1.433 (5) |
| C6—C11 | 1.477 (5) | C21—Fe3 | 2.068 (4) |
| C6—Fe1 | 2.065 (4) | C22—C23 | 1.402 (6) |
| C7—C8 | 1.415 (5) | C22—Fe3 | 2.036 (4) |
| C7—Fe1 | 2.052 (4) | C22—H22 | 0.9800 |
| C7—H7 | 0.9800 | C23—C24 | 1.403 (6) |
| C8—C9 | 1.404 (6) | C23—Fe3 | 2.029 (4) |
| C8—Fe1 | 2.024 (4) | C23—H23 | 0.9800 |
| C8—H8 | 0.9800 | C24—C25 | 1.414 (5) |
| C9—C10 | 1.396 (5) | C24—Fe3 | 2.029 (4) |
| C9—Fe1 | 2.016 (4) | C24—H24 | 0.9800 |
| C9—H9 | 0.9800 | C25—Fe3 | 2.059 (4) |
| C10—Fe1 | 2.032 (4) | C25—H25 | 0.9800 |
| C10—H10 | 0.9800 | C26—C27 | 1.404 (5) |
| C11—C15 | 1.411 (5) | C26—C30 | 1.432 (5) |
| C11—C12 | 1.427 (5) | C26—Fe3 | 2.072 (4) |
| C11—Fe2 | 2.063 (4) | C27—C28 | 1.413 (5) |
| C12—C13 | 1.411 (5) | C27—Fe3 | 2.055 (4) |
| C12—Fe2 | 2.031 (4) | C27—H27 | 0.9800 |
| C12—H12 | 0.9800 | C28—C29 | 1.396 (6) |
| C13—C14 | 1.398 (6) | C28—Fe3 | 2.032 (4) |
| C13—Fe2 | 2.023 (4) | C28—H28 | 0.9800 |
| C13—H13 | 0.9800 | C29—C30 | 1.416 (6) |
| C14—C15 | 1.413 (5) | C29—Fe3 | 2.033 (4) |
| C14—Fe2 | 2.028 (4) | C29—H29 | 0.9800 |
| C14—H14 | 0.9800 | C30—Fe3 | 2.033 (4) |
| C15—Fe2 | 2.051 (4) | C30—H30 | 0.9800 |
| C15—H15 | 0.9800 | | |

| | | | |
|---|---|---|---|
| C5—C1—C2 | 107.2 (3) | C28—C27—Fe3 | 68.9 (2) |
| C5—C1—C26 | 128.8 (4) | C26—C27—H27 | 125.7 |
| C2—C1—C26 | 123.5 (4) | C28—C27—H27 | 125.7 |
| C5—C1—Fe1 | 69.6 (2) | Fe3—C27—H27 | 125.7 |
| C2—C1—Fe1 | 68.9 (2) | C29—C28—C27 | 108.3 (4) |

| | | | |
|---|---|---|---|
| C26—C1—Fe1 | 132.3 (3) | C29—C28—Fe3 | 70.0 (3) |
| C3—C2—C1 | 107.1 (4) | C27—C28—Fe3 | 70.7 (2) |
| C3—C2—Fe1 | 68.4 (2) | C29—C28—H28 | 125.8 |
| C1—C2—Fe1 | 70.1 (2) | C27—C28—H28 | 125.8 |
| C3—C2—H2 | 126.5 | Fe3—C28—H28 | 125.8 |
| C1—C2—H2 | 126.5 | C28—C29—C30 | 108.2 (4) |
| Fe1—C2—H2 | 126.5 | C28—C29—Fe3 | 69.8 (2) |
| C4—C3—C2 | 108.8 (4) | C30—C29—Fe3 | 69.6 (2) |
| C4—C3—Fe1 | 70.5 (2) | C28—C29—H29 | 125.9 |
| C2—C3—Fe1 | 70.6 (2) | C30—C29—H29 | 125.9 |
| C4—C3—H3 | 125.6 | Fe3—C29—H29 | 125.9 |
| C2—C3—H3 | 125.6 | C29—C30—C26 | 107.6 (4) |
| Fe1—C3—H3 | 125.6 | C29—C30—Fe3 | 69.6 (2) |
| C3—C4—C5 | 107.9 (4) | C26—C30—Fe3 | 71.1 (2) |
| C3—C4—Fe1 | 68.9 (3) | C29—C30—H30 | 126.2 |
| C5—C4—Fe1 | 70.4 (2) | C26—C30—H30 | 126.2 |
| C3—C4—H4 | 126.1 | Fe3—C30—H30 | 126.2 |
| C5—C4—H4 | 126.1 | C9—Fe1—C3 | 102.26 (17) |
| Fe1—C4—H4 | 126.1 | C9—Fe1—C8 | 40.68 (17) |
| C4—C5—C1 | 109.0 (4) | C3—Fe1—C8 | 119.35 (18) |
| C4—C5—Fe1 | 69.2 (2) | C9—Fe1—C10 | 40.33 (15) |
| C1—C5—Fe1 | 70.2 (2) | C3—Fe1—C10 | 118.61 (16) |
| C4—C5—H5 | 125.5 | C8—Fe1—C10 | 67.99 (18) |
| C1—C5—H5 | 125.5 | C9—Fe1—C4 | 119.14 (19) |
| Fe1—C5—H5 | 125.5 | C3—Fe1—C4 | 40.58 (15) |
| C7—C6—C10 | 106.2 (4) | C8—Fe1—C4 | 155.12 (17) |
| C7—C6—C11 | 128.7 (3) | C10—Fe1—C4 | 106.03 (17) |
| C10—C6—C11 | 124.7 (4) | C9—Fe1—C2 | 118.76 (17) |
| C7—C6—Fe1 | 69.4 (2) | C3—Fe1—C2 | 40.98 (15) |
| C10—C6—Fe1 | 68.4 (2) | C8—Fe1—C2 | 105.85 (17) |
| C11—C6—Fe1 | 132.1 (3) | C10—Fe1—C2 | 154.35 (15) |
| C6—C7—C8 | 108.7 (4) | C4—Fe1—C2 | 68.55 (17) |
| C6—C7—Fe1 | 70.4 (2) | C9—Fe1—C7 | 68.13 (17) |
| C8—C7—Fe1 | 68.7 (2) | C3—Fe1—C7 | 157.90 (17) |
| C6—C7—H7 | 125.6 | C8—Fe1—C7 | 40.63 (14) |
| C8—C7—H7 | 125.6 | C10—Fe1—C7 | 67.65 (16) |
| Fe1—C7—H7 | 125.6 | C4—Fe1—C7 | 161.48 (16) |
| C9—C8—C7 | 107.8 (4) | C2—Fe1—C7 | 124.82 (17) |
| C9—C8—Fe1 | 69.4 (3) | C9—Fe1—C5 | 157.23 (19) |
| C7—C8—Fe1 | 70.7 (2) | C3—Fe1—C5 | 68.08 (16) |
| C9—C8—H8 | 126.1 | C8—Fe1—C5 | 162.02 (18) |
| C7—C8—H8 | 126.1 | C10—Fe1—C5 | 124.78 (17) |
| Fe1—C8—H8 | 126.1 | C4—Fe1—C5 | 40.37 (14) |
| C10—C9—C8 | 108.2 (4) | C2—Fe1—C5 | 68.22 (16) |
| C10—C9—Fe1 | 70.5 (2) | C7—Fe1—C5 | 127.87 (15) |
| C8—C9—Fe1 | 70.0 (2) | C9—Fe1—C1 | 157.37 (18) |
| C10—C9—H9 | 125.9 | C3—Fe1—C1 | 68.77 (15) |
| C8—C9—H9 | 125.9 | C8—Fe1—C1 | 124.38 (18) |

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|---|---|---|---|
| Fe1—C9—H9 | 125.9 | C10—Fe1—C1 | 162.19 (16) |
| C9—C10—C6 | 109.0 (4) | C4—Fe1—C1 | 68.23 (16) |
| C9—C10—Fe1 | 69.2 (2) | C2—Fe1—C1 | 41.09 (13) |
| C6—C10—Fe1 | 70.9 (2) | C7—Fe1—C1 | 112.16 (15) |
| C9—C10—H10 | 125.5 | C5—Fe1—C1 | 40.18 (14) |
| C6—C10—H10 | 125.5 | C9—Fe1—C6 | 68.54 (16) |
| Fe1—C10—H10 | 125.5 | C3—Fe1—C6 | 156.58 (17) |
| C15—C11—C12 | 107.0 (3) | C8—Fe1—C6 | 68.43 (16) |
| C15—C11—C6 | 127.6 (4) | C10—Fe1—C6 | 40.75 (13) |
| C12—C11—C6 | 125.1 (4) | C4—Fe1—C6 | 123.77 (17) |
| C15—C11—Fe2 | 69.5 (2) | C2—Fe1—C6 | 162.32 (16) |
| C12—C11—Fe2 | 68.4 (2) | C7—Fe1—C6 | 40.21 (14) |
| C6—C11—Fe2 | 132.0 (3) | C5—Fe1—C6 | 111.81 (15) |
| C13—C12—C11 | 108.0 (4) | C1—Fe1—C6 | 127.38 (14) |
| C13—C12—Fe2 | 69.3 (2) | C19—Fe2—C13 | 101.05 (17) |
| C11—C12—Fe2 | 70.8 (2) | C19—Fe2—C14 | 116.93 (18) |
| C13—C12—H12 | 126.0 | C13—Fe2—C14 | 40.38 (16) |
| C11—C12—H12 | 126.0 | C19—Fe2—C20 | 40.91 (15) |
| Fe2—C12—H12 | 126.0 | C13—Fe2—C20 | 117.94 (16) |
| C14—C13—C12 | 108.3 (4) | C14—Fe2—C20 | 104.36 (17) |
| C14—C13—Fe2 | 70.0 (2) | C19—Fe2—C12 | 118.90 (17) |
| C12—C13—Fe2 | 69.9 (2) | C13—Fe2—C12 | 40.75 (15) |
| C14—C13—H13 | 125.8 | C14—Fe2—C12 | 68.28 (17) |
| C12—C13—H13 | 125.8 | C20—Fe2—C12 | 154.47 (16) |
| Fe2—C13—H13 | 125.8 | C19—Fe2—C18 | 40.33 (15) |
| C13—C14—C15 | 108.1 (4) | C13—Fe2—C18 | 118.12 (18) |
| C13—C14—Fe2 | 69.6 (3) | C14—Fe2—C18 | 152.70 (18) |
| C15—C14—Fe2 | 70.6 (2) | C20—Fe2—C18 | 68.23 (17) |
| C13—C14—H14 | 125.9 | C12—Fe2—C18 | 106.54 (17) |
| C15—C14—H14 | 125.9 | C19—Fe2—C15 | 155.19 (18) |
| Fe2—C14—H14 | 125.9 | C13—Fe2—C15 | 67.94 (17) |
| C11—C15—C14 | 108.5 (4) | C14—Fe2—C15 | 40.54 (14) |
| C11—C15—Fe2 | 70.4 (2) | C20—Fe2—C15 | 123.15 (17) |
| C14—C15—Fe2 | 68.9 (2) | C12—Fe2—C15 | 67.98 (16) |
| C11—C15—H15 | 125.7 | C18—Fe2—C15 | 164.46 (16) |
| C14—C15—H15 | 125.7 | C19—Fe2—C17 | 67.76 (17) |
| Fe2—C15—H15 | 125.7 | C13—Fe2—C17 | 156.68 (18) |
| C17—C16—C20 | 106.7 (3) | C14—Fe2—C17 | 162.89 (17) |
| C17—C16—C21 | 128.2 (4) | C20—Fe2—C17 | 67.73 (16) |
| C20—C16—C21 | 124.3 (4) | C12—Fe2—C17 | 125.41 (17) |
| C17—C16—Fe2 | 69.7 (2) | C18—Fe2—C17 | 40.37 (14) |
| C20—C16—Fe2 | 68.3 (2) | C15—Fe2—C17 | 130.10 (16) |
| C21—C16—Fe2 | 134.5 (3) | C19—Fe2—C11 | 158.03 (17) |
| C16—C17—C18 | 109.0 (4) | C13—Fe2—C11 | 68.38 (15) |
| C16—C17—Fe2 | 70.3 (2) | C14—Fe2—C11 | 68.14 (16) |
| C18—C17—Fe2 | 69.2 (2) | C20—Fe2—C11 | 161.05 (17) |
| C16—C17—H17 | 125.5 | C12—Fe2—C11 | 40.79 (13) |
| C18—C17—H17 | 125.5 | C18—Fe2—C11 | 126.42 (17) |

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| Fe2—C17—H17 | 125.5 | C15—Fe2—C11 | 40.11 (14) |
| C19—C18—C17 | 107.7 (4) | C17—Fe2—C11 | 114.23 (15) |
| C19—C18—Fe2 | 69.0 (3) | C19—Fe2—C16 | 68.55 (16) |
| C17—C18—Fe2 | 70.4 (2) | C13—Fe2—C16 | 156.63 (17) |
| C19—C18—H18 | 126.1 | C14—Fe2—C16 | 124.27 (17) |
| C17—C18—H18 | 126.1 | C20—Fe2—C16 | 40.78 (13) |
| Fe2—C18—H18 | 126.1 | C12—Fe2—C16 | 162.57 (16) |
| C18—C19—C20 | 108.4 (4) | C18—Fe2—C16 | 68.13 (16) |
| C18—C19—Fe2 | 70.7 (2) | C15—Fe2—C16 | 112.50 (16) |
| C20—C19—Fe2 | 70.0 (2) | C17—Fe2—C16 | 40.02 (14) |
| C18—C19—H19 | 125.8 | C11—Fe2—C16 | 128.15 (15) |
| C20—C19—H19 | 125.8 | C23—Fe3—C24 | 40.45 (17) |
| Fe2—C19—H19 | 125.8 | C23—Fe3—C28 | 116.96 (19) |
| C19—C20—C16 | 108.1 (4) | C24—Fe3—C28 | 151.84 (18) |
| C19—C20—Fe2 | 69.1 (2) | C23—Fe3—C30 | 119.96 (17) |
| C16—C20—Fe2 | 71.0 (2) | C24—Fe3—C30 | 105.80 (18) |
| C19—C20—H20 | 126.0 | C28—Fe3—C30 | 68.19 (18) |
| C16—C20—H20 | 126.0 | C23—Fe3—C29 | 101.86 (17) |
| Fe2—C20—H20 | 126.0 | C24—Fe3—C29 | 117.27 (19) |
| C25—C21—C22 | 106.5 (4) | C28—Fe3—C29 | 40.18 (17) |
| C25—C21—C16 | 128.6 (4) | C30—Fe3—C29 | 40.77 (16) |
| C22—C21—C16 | 124.2 (4) | C23—Fe3—C22 | 40.35 (17) |
| C25—C21—Fe3 | 69.6 (2) | C24—Fe3—C22 | 67.78 (19) |
| C22—C21—Fe3 | 68.4 (2) | C28—Fe3—C22 | 106.07 (18) |
| C16—C21—Fe3 | 133.9 (3) | C30—Fe3—C22 | 156.22 (16) |
| C23—C22—C21 | 108.8 (4) | C29—Fe3—C22 | 120.04 (16) |
| C23—C22—Fe3 | 69.5 (2) | C23—Fe3—C27 | 154.7 (2) |
| C21—C22—Fe3 | 70.8 (2) | C24—Fe3—C27 | 164.80 (18) |
| C23—C22—H22 | 125.6 | C28—Fe3—C27 | 40.45 (14) |
| C21—C22—H22 | 125.6 | C30—Fe3—C27 | 67.91 (16) |
| Fe3—C22—H22 | 125.6 | C29—Fe3—C27 | 67.70 (17) |
| C22—C23—C24 | 107.9 (4) | C22—Fe3—C27 | 123.60 (18) |
| C22—C23—Fe3 | 70.1 (2) | C23—Fe3—C25 | 67.98 (17) |
| C24—C23—Fe3 | 69.8 (2) | C24—Fe3—C25 | 40.46 (15) |
| C22—C23—H23 | 126.1 | C28—Fe3—C25 | 164.75 (18) |
| C24—C23—H23 | 126.1 | C30—Fe3—C25 | 123.24 (18) |
| Fe3—C23—H23 | 126.1 | C29—Fe3—C25 | 155.06 (19) |
| C23—C24—C25 | 108.5 (4) | C22—Fe3—C25 | 67.67 (17) |
| C23—C24—Fe3 | 69.8 (3) | C27—Fe3—C25 | 130.43 (16) |
| C25—C24—Fe3 | 70.9 (2) | C23—Fe3—C21 | 68.45 (16) |
| C23—C24—H24 | 125.8 | C24—Fe3—C21 | 68.07 (16) |
| C25—C24—H24 | 125.8 | C28—Fe3—C21 | 126.28 (19) |
| Fe3—C24—H24 | 125.8 | C30—Fe3—C21 | 160.14 (16) |
| C21—C25—C24 | 108.4 (4) | C29—Fe3—C21 | 159.06 (18) |
| C21—C25—Fe3 | 70.3 (2) | C22—Fe3—C21 | 40.85 (14) |
| C24—C25—Fe3 | 68.6 (2) | C27—Fe3—C21 | 112.88 (16) |
| C21—C25—H25 | 125.8 | C25—Fe3—C21 | 40.05 (15) |
| C24—C25—H25 | 125.8 | C23—Fe3—C26 | 159.29 (18) |

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| Fe3—C25—H25 | 125.8 | C24—Fe3—C26 | 126.64 (18) |
| C27—C26—C30 | 107.3 (4) | C28—Fe3—C26 | 67.72 (16) |
| C27—C26—C1 | 128.1 (4) | C30—Fe3—C26 | 40.82 (14) |
| C30—C26—C1 | 124.2 (4) | C29—Fe3—C26 | 68.09 (15) |
| C27—C26—Fe3 | 69.5 (2) | C22—Fe3—C26 | 160.35 (17) |
| C30—C26—Fe3 | 68.1 (2) | C27—Fe3—C26 | 39.77 (14) |
| C1—C26—Fe3 | 133.4 (3) | C25—Fe3—C26 | 113.23 (16) |
| C26—C27—C28 | 108.6 (4) | C21—Fe3—C26 | 126.79 (14) |
| C26—C27—Fe3 | 70.8 (2) | | |

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| C5—C1—C2—C3 | 0.6 (4) | C14—C13—Fe2—C20 | −79.0 (3) |
| C26—C1—C2—C3 | 173.9 (4) | C12—C13—Fe2—C20 | 161.7 (2) |
| Fe1—C1—C2—C3 | −58.6 (3) | C14—C13—Fe2—C12 | 119.3 (4) |
| C5—C1—C2—Fe1 | 59.2 (3) | C14—C13—Fe2—C18 | −157.9 (2) |
| C26—C1—C2—Fe1 | −127.5 (4) | C12—C13—Fe2—C18 | 82.8 (3) |
| C1—C2—C3—C4 | −0.8 (5) | C14—C13—Fe2—C15 | 37.9 (2) |
| Fe1—C2—C3—C4 | −60.5 (3) | C12—C13—Fe2—C15 | −81.4 (3) |
| C1—C2—C3—Fe1 | 59.6 (3) | C14—C13—Fe2—C17 | −177.5 (3) |
| C2—C3—C4—C5 | 0.7 (5) | C12—C13—Fe2—C17 | 63.2 (5) |
| Fe1—C3—C4—C5 | −59.8 (3) | C14—C13—Fe2—C11 | 81.3 (3) |
| C2—C3—C4—Fe1 | 60.5 (3) | C12—C13—Fe2—C11 | −38.0 (2) |
| C3—C4—C5—C1 | −0.3 (5) | C14—C13—Fe2—C16 | −58.0 (5) |
| Fe1—C4—C5—C1 | −59.1 (3) | C12—C13—Fe2—C16 | −177.3 (4) |
| C3—C4—C5—Fe1 | 58.9 (3) | C13—C14—Fe2—C19 | 74.6 (3) |
| C2—C1—C5—C4 | −0.2 (4) | C15—C14—Fe2—C19 | −166.5 (2) |
| C26—C1—C5—C4 | −173.0 (4) | C15—C14—Fe2—C13 | 118.9 (4) |
| Fe1—C1—C5—C4 | 58.5 (3) | C13—C14—Fe2—C20 | 116.4 (3) |
| C2—C1—C5—Fe1 | −58.8 (3) | C15—C14—Fe2—C20 | −124.7 (2) |
| C26—C1—C5—Fe1 | 128.5 (4) | C13—C14—Fe2—C12 | −37.8 (2) |
| C10—C6—C7—C8 | −0.6 (4) | C15—C14—Fe2—C12 | 81.1 (2) |
| C11—C6—C7—C8 | −173.8 (4) | C13—C14—Fe2—C18 | 46.2 (5) |
| Fe1—C6—C7—C8 | 58.1 (3) | C15—C14—Fe2—C18 | 165.1 (3) |
| C10—C6—C7—Fe1 | −58.7 (3) | C13—C14—Fe2—C15 | −118.9 (4) |
| C11—C6—C7—Fe1 | 128.0 (4) | C13—C14—Fe2—C17 | 176.6 (5) |
| C6—C7—C8—C9 | 0.5 (5) | C15—C14—Fe2—C17 | −64.5 (6) |
| Fe1—C7—C8—C9 | 59.7 (3) | C13—C14—Fe2—C11 | −81.9 (3) |
| C6—C7—C8—Fe1 | −59.2 (3) | C15—C14—Fe2—C11 | 37.0 (2) |
| C7—C8—C9—C10 | −0.2 (5) | C13—C14—Fe2—C16 | 156.0 (2) |
| Fe1—C8—C9—C10 | 60.4 (3) | C15—C14—Fe2—C16 | −85.2 (3) |
| C7—C8—C9—Fe1 | −60.5 (3) | C16—C20—Fe2—C19 | −118.9 (4) |
| C8—C9—C10—C6 | −0.2 (5) | C19—C20—Fe2—C13 | −73.7 (3) |
| Fe1—C9—C10—C6 | 59.9 (3) | C16—C20—Fe2—C13 | 167.4 (3) |
| C8—C9—C10—Fe1 | −60.1 (3) | C19—C20—Fe2—C14 | −114.7 (3) |
| C7—C6—C10—C9 | 0.5 (5) | C16—C20—Fe2—C14 | 126.4 (3) |
| C11—C6—C10—C9 | 174.1 (4) | C19—C20—Fe2—C12 | −45.3 (5) |
| Fe1—C6—C10—C9 | −58.9 (3) | C16—C20—Fe2—C12 | −164.1 (4) |
| C7—C6—C10—Fe1 | 59.3 (3) | C19—C20—Fe2—C18 | 37.6 (3) |
| C11—C6—C10—Fe1 | −127.1 (4) | C16—C20—Fe2—C18 | −81.3 (3) |

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| C7—C6—C11—C15 | −106.9 (5) | C19—C20—Fe2—C15 | −154.4 (3) |
| C10—C6—C11—C15 | 81.0 (5) | C16—C20—Fe2—C15 | 86.7 (3) |
| Fe1—C6—C11—C15 | −10.2 (6) | C19—C20—Fe2—C17 | 81.3 (3) |
| C7—C6—C11—C12 | 80.3 (5) | C16—C20—Fe2—C17 | −37.6 (2) |
| C10—C6—C11—C12 | −91.8 (5) | C19—C20—Fe2—C11 | −178.8 (4) |
| Fe1—C6—C11—C12 | 176.9 (3) | C16—C20—Fe2—C11 | 62.3 (6) |
| C7—C6—C11—Fe2 | −11.3 (6) | C19—C20—Fe2—C16 | 118.9 (4) |
| C10—C6—C11—Fe2 | 176.6 (3) | C13—C12—Fe2—C19 | −72.2 (3) |
| Fe1—C6—C11—Fe2 | 85.4 (5) | C11—C12—Fe2—C19 | 169.0 (3) |
| C15—C11—C12—C13 | −0.6 (4) | C11—C12—Fe2—C13 | −118.7 (4) |
| C6—C11—C12—C13 | 173.4 (4) | C13—C12—Fe2—C14 | 37.5 (3) |
| Fe2—C11—C12—C13 | −59.6 (3) | C11—C12—Fe2—C14 | −81.3 (3) |
| C15—C11—C12—Fe2 | 58.9 (3) | C13—C12—Fe2—C20 | −40.1 (5) |
| C6—C11—C12—Fe2 | −127.0 (4) | C11—C12—Fe2—C20 | −158.9 (4) |
| C11—C12—C13—C14 | 0.8 (5) | C13—C12—Fe2—C18 | −114.1 (3) |
| Fe2—C12—C13—C14 | −59.7 (3) | C11—C12—Fe2—C18 | 127.1 (3) |
| C11—C12—C13—Fe2 | 60.5 (3) | C13—C12—Fe2—C15 | 81.3 (3) |
| C12—C13—C14—C15 | −0.7 (5) | C11—C12—Fe2—C15 | −37.4 (2) |
| Fe2—C13—C14—C15 | −60.3 (3) | C13—C12—Fe2—C17 | −154.3 (3) |
| C12—C13—C14—Fe2 | 59.7 (3) | C11—C12—Fe2—C17 | 87.0 (3) |
| C12—C11—C15—C14 | 0.2 (4) | C13—C12—Fe2—C11 | 118.7 (4) |
| C6—C11—C15—C14 | −173.6 (3) | C13—C12—Fe2—C16 | 176.4 (5) |
| Fe2—C11—C15—C14 | 58.5 (3) | C11—C12—Fe2—C16 | 57.7 (6) |
| C12—C11—C15—Fe2 | −58.3 (3) | C17—C18—Fe2—C19 | 118.9 (4) |
| C6—C11—C15—Fe2 | 127.9 (4) | C19—C18—Fe2—C13 | 72.9 (3) |
| C13—C14—C15—C11 | 0.3 (5) | C17—C18—Fe2—C13 | −168.2 (2) |
| Fe2—C14—C15—C11 | −59.4 (3) | C19—C18—Fe2—C14 | 40.9 (5) |
| C13—C14—C15—Fe2 | 59.7 (3) | C17—C18—Fe2—C14 | 159.7 (3) |
| C20—C16—C17—C18 | 0.1 (4) | C19—C18—Fe2—C20 | −38.1 (2) |
| C21—C16—C17—C18 | −170.3 (4) | C17—C18—Fe2—C20 | 80.8 (2) |
| Fe2—C16—C17—C18 | 58.5 (3) | C19—C18—Fe2—C12 | 115.4 (3) |
| C20—C16—C17—Fe2 | −58.4 (3) | C17—C18—Fe2—C12 | −125.7 (2) |
| C21—C16—C17—Fe2 | 131.3 (4) | C19—C18—Fe2—C15 | −177.7 (5) |
| C16—C17—C18—C19 | 0.0 (4) | C17—C18—Fe2—C15 | −58.8 (7) |
| Fe2—C17—C18—C19 | 59.1 (3) | C19—C18—Fe2—C17 | −118.9 (4) |
| C16—C17—C18—Fe2 | −59.1 (3) | C19—C18—Fe2—C11 | 155.7 (2) |
| C17—C18—C19—C20 | 0.0 (4) | C17—C18—Fe2—C11 | −85.4 (3) |
| Fe2—C18—C19—C20 | 60.0 (3) | C19—C18—Fe2—C16 | −82.2 (3) |
| C17—C18—C19—Fe2 | −60.0 (3) | C17—C18—Fe2—C16 | 36.7 (2) |
| C18—C19—C20—C16 | 0.1 (5) | C11—C15—Fe2—C19 | 149.6 (4) |
| Fe2—C19—C20—C16 | 60.5 (3) | C14—C15—Fe2—C19 | 29.7 (5) |
| C18—C19—C20—Fe2 | −60.5 (3) | C11—C15—Fe2—C13 | 82.2 (2) |
| C17—C16—C20—C19 | −0.1 (4) | C14—C15—Fe2—C13 | −37.7 (2) |
| C21—C16—C20—C19 | 170.7 (4) | C11—C15—Fe2—C14 | 119.9 (3) |
| Fe2—C16—C20—C19 | −59.4 (3) | C11—C15—Fe2—C20 | −168.0 (2) |
| C17—C16—C20—Fe2 | 59.3 (3) | C14—C15—Fe2—C20 | 72.1 (3) |
| C21—C16—C20—Fe2 | −129.9 (4) | C11—C15—Fe2—C12 | 38.1 (2) |
| C17—C16—C21—C25 | −117.0 (5) | C14—C15—Fe2—C12 | −81.9 (3) |

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| C20—C16—C21—C25 | 74.3 (5) | C11—C15—Fe2—C18 | −34.0 (7) |
| Fe2—C16—C21—C25 | −18.1 (7) | C14—C15—Fe2—C18 | −153.9 (6) |
| C17—C16—C21—C22 | 73.7 (5) | C11—C15—Fe2—C17 | −80.4 (3) |
| C20—C16—C21—C22 | −95.1 (5) | C14—C15—Fe2—C17 | 159.7 (2) |
| Fe2—C16—C21—C22 | 172.6 (3) | C14—C15—Fe2—C11 | −119.9 (3) |
| C17—C16—C21—Fe3 | −18.4 (6) | C11—C15—Fe2—C16 | −123.1 (2) |
| C20—C16—C21—Fe3 | 172.9 (3) | C14—C15—Fe2—C16 | 117.0 (3) |
| Fe2—C16—C21—Fe3 | 80.5 (5) | C16—C17—Fe2—C19 | 82.7 (2) |
| C25—C21—C22—C23 | 0.1 (5) | C18—C17—Fe2—C19 | −37.8 (2) |
| C16—C21—C22—C23 | 171.5 (4) | C16—C17—Fe2—C13 | 147.5 (4) |
| Fe3—C21—C22—C23 | −59.4 (3) | C18—C17—Fe2—C13 | 27.1 (5) |
| C25—C21—C22—Fe3 | 59.5 (3) | C16—C17—Fe2—C14 | −26.9 (6) |
| C16—C21—C22—Fe3 | −129.2 (4) | C18—C17—Fe2—C14 | −147.3 (5) |
| C21—C22—C23—C24 | 0.3 (5) | C16—C17—Fe2—C20 | 38.3 (2) |
| Fe3—C22—C23—C24 | −59.8 (3) | C18—C17—Fe2—C20 | −82.1 (2) |
| C21—C22—C23—Fe3 | 60.1 (3) | C16—C17—Fe2—C12 | −166.8 (2) |
| C22—C23—C24—C25 | −0.6 (5) | C18—C17—Fe2—C12 | 72.7 (3) |
| Fe3—C23—C24—C25 | −60.6 (3) | C16—C17—Fe2—C18 | 120.4 (3) |
| C22—C23—C24—Fe3 | 60.0 (3) | C16—C17—Fe2—C15 | −77.0 (3) |
| C22—C21—C25—C24 | −0.5 (4) | C18—C17—Fe2—C15 | 162.6 (2) |
| C16—C21—C25—C24 | −171.3 (4) | C16—C17—Fe2—C11 | −121.2 (2) |
| Fe3—C21—C25—C24 | 58.2 (3) | C18—C17—Fe2—C11 | 118.4 (2) |
| C22—C21—C25—Fe3 | −58.7 (3) | C18—C17—Fe2—C16 | −120.4 (3) |
| C16—C21—C25—Fe3 | 130.5 (4) | C15—C11—Fe2—C19 | −145.4 (4) |
| C23—C24—C25—C21 | 0.6 (5) | C12—C11—Fe2—C19 | −26.4 (6) |
| Fe3—C24—C25—C21 | −59.3 (3) | C6—C11—Fe2—C19 | 91.9 (6) |
| C23—C24—C25—Fe3 | 59.9 (3) | C15—C11—Fe2—C13 | −81.0 (3) |
| C5—C1—C26—C27 | −109.1 (5) | C12—C11—Fe2—C13 | 38.0 (3) |
| C2—C1—C26—C27 | 79.2 (5) | C6—C11—Fe2—C13 | 156.4 (4) |
| Fe1—C1—C26—C27 | −11.9 (6) | C15—C11—Fe2—C14 | −37.4 (2) |
| C5—C1—C26—C30 | 79.4 (5) | C12—C11—Fe2—C14 | 81.6 (3) |
| C2—C1—C26—C30 | −92.2 (5) | C6—C11—Fe2—C14 | −160.0 (4) |
| Fe1—C1—C26—C30 | 176.7 (3) | C15—C11—Fe2—C20 | 32.4 (6) |
| C5—C1—C26—Fe3 | −11.8 (7) | C12—C11—Fe2—C20 | 151.4 (5) |
| C2—C1—C26—Fe3 | 176.5 (3) | C6—C11—Fe2—C20 | −90.2 (6) |
| Fe1—C1—C26—Fe3 | 85.5 (5) | C15—C11—Fe2—C12 | −119.0 (3) |
| C30—C26—C27—C28 | 0.9 (4) | C6—C11—Fe2—C12 | 118.4 (5) |
| C1—C26—C27—C28 | −171.6 (4) | C15—C11—Fe2—C18 | 169.3 (2) |
| Fe3—C26—C27—C28 | 58.7 (3) | C12—C11—Fe2—C18 | −71.7 (3) |
| C30—C26—C27—Fe3 | −57.8 (3) | C6—C11—Fe2—C18 | 46.7 (4) |
| C1—C26—C27—Fe3 | 129.6 (4) | C12—C11—Fe2—C15 | 119.0 (3) |
| C26—C27—C28—C29 | 0.2 (5) | C6—C11—Fe2—C15 | −122.6 (5) |
| Fe3—C27—C28—C29 | 60.1 (3) | C15—C11—Fe2—C17 | 124.2 (2) |
| C26—C27—C28—Fe3 | −59.9 (3) | C12—C11—Fe2—C17 | −116.8 (3) |
| C27—C28—C29—C30 | −1.3 (5) | C6—C11—Fe2—C17 | 1.6 (4) |
| Fe3—C28—C29—C30 | 59.2 (3) | C15—C11—Fe2—C16 | 79.8 (3) |
| C27—C28—C29—Fe3 | −60.5 (3) | C12—C11—Fe2—C16 | −161.2 (2) |
| C28—C29—C30—C26 | 1.8 (5) | C6—C11—Fe2—C16 | −42.8 (5) |

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| Fe3—C29—C30—C26 | 61.2 (3) | C17—C16—Fe2—C19 | −80.5 (3) |
| C28—C29—C30—Fe3 | −59.4 (3) | C20—C16—Fe2—C19 | 38.0 (3) |
| C27—C26—C30—C29 | −1.7 (4) | C21—C16—Fe2—C19 | 155.3 (5) |
| C1—C26—C30—C29 | 171.2 (4) | C17—C16—Fe2—C13 | −147.6 (4) |
| Fe3—C26—C30—C29 | −60.3 (3) | C20—C16—Fe2—C13 | −29.0 (5) |
| C27—C26—C30—Fe3 | 58.6 (3) | C21—C16—Fe2—C13 | 88.3 (6) |
| C1—C26—C30—Fe3 | −128.5 (4) | C17—C16—Fe2—C14 | 170.7 (2) |
| C10—C9—Fe1—C3 | 120.1 (3) | C20—C16—Fe2—C14 | −70.7 (3) |
| C8—C9—Fe1—C3 | −121.1 (3) | C21—C16—Fe2—C14 | 46.6 (5) |
| C10—C9—Fe1—C8 | −118.8 (4) | C17—C16—Fe2—C20 | −118.6 (3) |
| C8—C9—Fe1—C10 | 118.8 (4) | C21—C16—Fe2—C20 | 117.3 (5) |
| C10—C9—Fe1—C4 | 80.3 (3) | C17—C16—Fe2—C12 | 38.3 (6) |
| C8—C9—Fe1—C4 | −160.9 (2) | C20—C16—Fe2—C12 | 156.8 (5) |
| C10—C9—Fe1—C2 | 160.4 (3) | C21—C16—Fe2—C12 | −85.9 (7) |
| C8—C9—Fe1—C2 | −80.7 (3) | C17—C16—Fe2—C18 | −37.0 (2) |
| C10—C9—Fe1—C7 | −80.8 (3) | C20—C16—Fe2—C18 | 81.6 (3) |
| C8—C9—Fe1—C7 | 38.0 (2) | C21—C16—Fe2—C18 | −161.1 (5) |
| C10—C9—Fe1—C5 | 58.1 (5) | C17—C16—Fe2—C15 | 126.2 (2) |
| C8—C9—Fe1—C5 | 176.9 (4) | C20—C16—Fe2—C15 | −115.2 (3) |
| C10—C9—Fe1—C1 | −176.2 (4) | C21—C16—Fe2—C15 | 2.1 (5) |
| C8—C9—Fe1—C1 | −57.3 (5) | C20—C16—Fe2—C17 | 118.6 (3) |
| C10—C9—Fe1—C6 | −37.4 (3) | C21—C16—Fe2—C17 | −124.1 (5) |
| C8—C9—Fe1—C6 | 81.4 (3) | C17—C16—Fe2—C11 | 82.9 (3) |
| C4—C3—Fe1—C9 | −120.8 (3) | C20—C16—Fe2—C11 | −158.5 (3) |
| C2—C3—Fe1—C9 | 120.0 (3) | C21—C16—Fe2—C11 | −41.3 (5) |
| C4—C3—Fe1—C8 | −160.6 (2) | C22—C23—Fe3—C24 | −118.7 (4) |
| C2—C3—Fe1—C8 | 80.2 (3) | C22—C23—Fe3—C28 | 83.2 (3) |
| C4—C3—Fe1—C10 | −81.2 (3) | C24—C23—Fe3—C28 | −158.1 (3) |
| C2—C3—Fe1—C10 | 159.7 (2) | C22—C23—Fe3—C30 | 162.3 (3) |
| C2—C3—Fe1—C4 | −119.1 (3) | C24—C23—Fe3—C30 | −78.9 (3) |
| C4—C3—Fe1—C2 | 119.1 (3) | C22—C23—Fe3—C29 | 122.9 (3) |
| C4—C3—Fe1—C7 | 177.7 (4) | C24—C23—Fe3—C29 | −118.4 (3) |
| C2—C3—Fe1—C7 | 58.6 (5) | C24—C23—Fe3—C22 | 118.7 (4) |
| C4—C3—Fe1—C5 | 37.6 (2) | C22—C23—Fe3—C27 | 60.5 (5) |
| C2—C3—Fe1—C5 | −81.6 (3) | C24—C23—Fe3—C27 | 179.2 (3) |
| C4—C3—Fe1—C1 | 80.9 (2) | C22—C23—Fe3—C25 | −81.0 (3) |
| C2—C3—Fe1—C1 | −38.2 (2) | C24—C23—Fe3—C25 | 37.8 (2) |
| C4—C3—Fe1—C6 | −56.9 (5) | C22—C23—Fe3—C21 | −37.7 (3) |
| C2—C3—Fe1—C6 | −176.1 (4) | C24—C23—Fe3—C21 | 81.0 (3) |
| C7—C8—Fe1—C9 | 118.6 (4) | C22—C23—Fe3—C26 | −178.6 (4) |
| C9—C8—Fe1—C3 | 73.7 (3) | C24—C23—Fe3—C26 | −59.9 (6) |
| C7—C8—Fe1—C3 | −167.7 (2) | C25—C24—Fe3—C23 | 119.0 (4) |
| C9—C8—Fe1—C10 | −37.7 (2) | C23—C24—Fe3—C28 | 44.7 (5) |
| C7—C8—Fe1—C10 | 80.9 (2) | C25—C24—Fe3—C28 | 163.7 (3) |
| C9—C8—Fe1—C4 | 42.9 (5) | C23—C24—Fe3—C30 | 117.9 (3) |
| C7—C8—Fe1—C4 | 161.4 (3) | C25—C24—Fe3—C30 | −123.1 (3) |
| C9—C8—Fe1—C2 | 115.9 (3) | C23—C24—Fe3—C29 | 75.6 (3) |
| C7—C8—Fe1—C2 | −125.5 (2) | C25—C24—Fe3—C29 | −165.4 (2) |

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| C9—C8—Fe1—C7 | −118.6 (4) | C23—C24—Fe3—C22 | −37.8 (2) |
| C9—C8—Fe1—C5 | −176.1 (5) | C25—C24—Fe3—C22 | 81.2 (3) |
| C7—C8—Fe1—C5 | −57.5 (6) | C23—C24—Fe3—C27 | −178.8 (5) |
| C9—C8—Fe1—C1 | 156.9 (2) | C25—C24—Fe3—C27 | −59.8 (7) |
| C7—C8—Fe1—C1 | −84.5 (3) | C23—C24—Fe3—C25 | −119.0 (4) |
| C9—C8—Fe1—C6 | −81.8 (3) | C23—C24—Fe3—C21 | −82.1 (3) |
| C7—C8—Fe1—C6 | 36.8 (2) | C25—C24—Fe3—C21 | 36.9 (2) |
| C6—C10—Fe1—C9 | −120.1 (4) | C23—C24—Fe3—C26 | 157.6 (2) |
| C9—C10—Fe1—C3 | −74.4 (3) | C25—C24—Fe3—C26 | −83.4 (3) |
| C6—C10—Fe1—C3 | 165.5 (3) | C29—C28—Fe3—C23 | 75.8 (3) |
| C9—C10—Fe1—C8 | 38.0 (3) | C27—C28—Fe3—C23 | −165.3 (2) |
| C6—C10—Fe1—C8 | −82.0 (3) | C29—C28—Fe3—C24 | 45.0 (5) |
| C9—C10—Fe1—C4 | −116.4 (3) | C27—C28—Fe3—C24 | 163.8 (3) |
| C6—C10—Fe1—C4 | 123.5 (3) | C29—C28—Fe3—C30 | −37.8 (2) |
| C9—C10—Fe1—C2 | −42.7 (5) | C27—C28—Fe3—C30 | 81.1 (3) |
| C6—C10—Fe1—C2 | −162.8 (4) | C27—C28—Fe3—C29 | 118.9 (4) |
| C9—C10—Fe1—C7 | 82.1 (3) | C29—C28—Fe3—C22 | 117.8 (3) |
| C6—C10—Fe1—C7 | −38.0 (2) | C27—C28—Fe3—C22 | −123.3 (3) |
| C9—C10—Fe1—C5 | −156.4 (3) | C29—C28—Fe3—C27 | −118.9 (4) |
| C6—C10—Fe1—C5 | 83.5 (3) | C29—C28—Fe3—C25 | −178.7 (5) |
| C9—C10—Fe1—C1 | 175.2 (5) | C27—C28—Fe3—C25 | −59.9 (7) |
| C6—C10—Fe1—C1 | 55.1 (6) | C29—C28—Fe3—C21 | 157.9 (2) |
| C9—C10—Fe1—C6 | 120.1 (4) | C27—C28—Fe3—C21 | −83.3 (3) |
| C3—C4—Fe1—C9 | 73.9 (3) | C29—C28—Fe3—C26 | −82.0 (3) |
| C5—C4—Fe1—C9 | −166.9 (2) | C27—C28—Fe3—C26 | 36.9 (2) |
| C5—C4—Fe1—C3 | 119.2 (3) | C29—C30—Fe3—C23 | −72.2 (3) |
| C3—C4—Fe1—C8 | 43.4 (5) | C26—C30—Fe3—C23 | 169.8 (3) |
| C5—C4—Fe1—C8 | 162.6 (4) | C29—C30—Fe3—C24 | −113.6 (3) |
| C3—C4—Fe1—C10 | 115.5 (2) | C26—C30—Fe3—C24 | 128.4 (3) |
| C5—C4—Fe1—C10 | −125.3 (2) | C29—C30—Fe3—C28 | 37.2 (3) |
| C3—C4—Fe1—C2 | −38.0 (2) | C26—C30—Fe3—C28 | −80.7 (3) |
| C5—C4—Fe1—C2 | 81.2 (2) | C26—C30—Fe3—C29 | −118.0 (4) |
| C3—C4—Fe1—C7 | −177.3 (4) | C29—C30—Fe3—C22 | −43.1 (6) |
| C5—C4—Fe1—C7 | −58.2 (6) | C26—C30—Fe3—C22 | −161.0 (4) |
| C3—C4—Fe1—C5 | −119.2 (3) | C29—C30—Fe3—C27 | 81.0 (3) |
| C3—C4—Fe1—C1 | −82.3 (2) | C26—C30—Fe3—C27 | −36.9 (2) |
| C5—C4—Fe1—C1 | 36.8 (2) | C29—C30—Fe3—C25 | −154.2 (3) |
| C3—C4—Fe1—C6 | 156.4 (2) | C26—C30—Fe3—C25 | 87.9 (3) |
| C5—C4—Fe1—C6 | −84.5 (3) | C29—C30—Fe3—C21 | 177.4 (4) |
| C3—C2—Fe1—C9 | −74.8 (3) | C26—C30—Fe3—C21 | 59.5 (6) |
| C1—C2—Fe1—C9 | 166.6 (3) | C29—C30—Fe3—C26 | 118.0 (4) |
| C1—C2—Fe1—C3 | −118.7 (4) | C28—C29—Fe3—C23 | −118.0 (3) |
| C3—C2—Fe1—C8 | −116.7 (3) | C30—C29—Fe3—C23 | 122.6 (3) |
| C1—C2—Fe1—C8 | 124.6 (3) | C28—C29—Fe3—C24 | −158.0 (3) |
| C3—C2—Fe1—C10 | −44.7 (5) | C30—C29—Fe3—C24 | 82.6 (3) |
| C1—C2—Fe1—C10 | −163.4 (4) | C30—C29—Fe3—C28 | −119.4 (4) |
| C3—C2—Fe1—C4 | 37.6 (2) | C28—C29—Fe3—C30 | 119.4 (4) |
| C1—C2—Fe1—C4 | −81.0 (3) | C28—C29—Fe3—C22 | −79.1 (3) |

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| C3—C2—Fe1—C7 | −157.0 (2) | C30—C29—Fe3—C22 | 161.5 (3) |
| C1—C2—Fe1—C7 | 84.4 (3) | C28—C29—Fe3—C27 | 37.9 (2) |
| C3—C2—Fe1—C5 | 81.2 (3) | C30—C29—Fe3—C27 | −81.6 (3) |
| C1—C2—Fe1—C5 | −37.5 (2) | C28—C29—Fe3—C25 | 179.2 (3) |
| C3—C2—Fe1—C1 | 118.7 (4) | C30—C29—Fe3—C25 | 59.8 (5) |
| C3—C2—Fe1—C6 | 174.8 (5) | C28—C29—Fe3—C21 | −58.1 (6) |
| C1—C2—Fe1—C6 | 56.2 (6) | C30—C29—Fe3—C21 | −177.5 (4) |
| C6—C7—Fe1—C9 | 82.2 (3) | C28—C29—Fe3—C26 | 81.0 (3) |
| C8—C7—Fe1—C9 | −38.1 (2) | C30—C29—Fe3—C26 | −38.5 (2) |
| C6—C7—Fe1—C3 | 149.8 (4) | C21—C22—Fe3—C23 | −119.6 (4) |
| C8—C7—Fe1—C3 | 29.6 (5) | C23—C22—Fe3—C24 | 37.9 (3) |
| C6—C7—Fe1—C8 | 120.3 (3) | C21—C22—Fe3—C24 | −81.7 (3) |
| C6—C7—Fe1—C10 | 38.5 (2) | C23—C22—Fe3—C28 | −112.9 (3) |
| C8—C7—Fe1—C10 | −81.8 (3) | C21—C22—Fe3—C28 | 127.5 (3) |
| C6—C7—Fe1—C4 | −34.8 (6) | C23—C22—Fe3—C30 | −40.7 (6) |
| C8—C7—Fe1—C4 | −155.1 (4) | C21—C22—Fe3—C30 | −160.3 (4) |
| C6—C7—Fe1—C2 | −167.2 (2) | C23—C22—Fe3—C29 | −71.7 (4) |
| C8—C7—Fe1—C2 | 72.6 (3) | C21—C22—Fe3—C29 | 168.7 (3) |
| C6—C7—Fe1—C5 | −79.0 (3) | C23—C22—Fe3—C27 | −153.5 (3) |
| C8—C7—Fe1—C5 | 160.7 (3) | C21—C22—Fe3—C27 | 86.9 (3) |
| C6—C7—Fe1—C1 | −122.2 (2) | C23—C22—Fe3—C25 | 81.8 (3) |
| C8—C7—Fe1—C1 | 117.5 (3) | C21—C22—Fe3—C25 | −37.8 (2) |
| C8—C7—Fe1—C6 | −120.3 (3) | C23—C22—Fe3—C21 | 119.6 (4) |
| C4—C5—Fe1—C9 | 30.7 (5) | C23—C22—Fe3—C26 | 178.6 (4) |
| C1—C5—Fe1—C9 | 151.1 (4) | C21—C22—Fe3—C26 | 58.9 (6) |
| C4—C5—Fe1—C3 | −37.8 (2) | C26—C27—Fe3—C23 | 151.7 (4) |
| C1—C5—Fe1—C3 | 82.6 (2) | C28—C27—Fe3—C23 | 31.9 (5) |
| C4—C5—Fe1—C8 | −155.9 (5) | C26—C27—Fe3—C24 | −30.2 (7) |
| C1—C5—Fe1—C8 | −35.5 (6) | C28—C27—Fe3—C24 | −149.9 (6) |
| C4—C5—Fe1—C10 | 72.7 (3) | C26—C27—Fe3—C28 | 119.7 (4) |
| C1—C5—Fe1—C10 | −167.0 (2) | C26—C27—Fe3—C30 | 37.9 (2) |
| C1—C5—Fe1—C4 | 120.4 (3) | C28—C27—Fe3—C30 | −81.8 (3) |
| C4—C5—Fe1—C2 | −82.1 (2) | C26—C27—Fe3—C29 | 82.1 (3) |
| C1—C5—Fe1—C2 | 38.3 (2) | C28—C27—Fe3—C29 | −37.6 (3) |
| C4—C5—Fe1—C7 | 160.0 (2) | C26—C27—Fe3—C22 | −165.8 (2) |
| C1—C5—Fe1—C7 | −79.6 (3) | C28—C27—Fe3—C22 | 74.5 (3) |
| C4—C5—Fe1—C1 | −120.4 (3) | C26—C27—Fe3—C25 | −77.7 (3) |
| C4—C5—Fe1—C6 | 117.0 (2) | C28—C27—Fe3—C25 | 162.6 (3) |
| C1—C5—Fe1—C6 | −122.7 (2) | C26—C27—Fe3—C21 | −120.6 (2) |
| C5—C1—Fe1—C9 | −150.9 (4) | C28—C27—Fe3—C21 | 119.7 (3) |
| C2—C1—Fe1—C9 | −32.0 (6) | C28—C27—Fe3—C26 | −119.7 (4) |
| C26—C1—Fe1—C9 | 84.7 (6) | C21—C25—Fe3—C23 | 82.3 (3) |
| C5—C1—Fe1—C3 | −80.8 (3) | C24—C25—Fe3—C23 | −37.7 (3) |
| C2—C1—Fe1—C3 | 38.1 (2) | C21—C25—Fe3—C24 | 120.0 (4) |
| C26—C1—Fe1—C3 | 154.8 (4) | C21—C25—Fe3—C28 | −29.8 (7) |
| C5—C1—Fe1—C8 | 167.5 (2) | C24—C25—Fe3—C28 | −149.8 (6) |
| C2—C1—Fe1—C8 | −73.7 (3) | C21—C25—Fe3—C30 | −165.5 (2) |
| C26—C1—Fe1—C8 | 43.0 (4) | C24—C25—Fe3—C30 | 74.5 (3) |

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| C5—C1—Fe1—C10 | 37.3 (6) | C21—C25—Fe3—C29 | 152.1 (3) |
| C2—C1—Fe1—C10 | 156.2 (5) | C24—C25—Fe3—C29 | 32.1 (5) |
| C26—C1—Fe1—C10 | −87.1 (7) | C21—C25—Fe3—C22 | 38.5 (2) |
| C5—C1—Fe1—C4 | −37.0 (2) | C24—C25—Fe3—C22 | −81.5 (3) |
| C2—C1—Fe1—C4 | 81.9 (3) | C21—C25—Fe3—C27 | −77.3 (3) |
| C26—C1—Fe1—C4 | −161.4 (4) | C24—C25—Fe3—C27 | 162.7 (3) |
| C5—C1—Fe1—C2 | −118.9 (3) | C24—C25—Fe3—C21 | −120.0 (4) |
| C26—C1—Fe1—C2 | 116.7 (5) | C21—C25—Fe3—C26 | −120.2 (2) |
| C5—C1—Fe1—C7 | 123.0 (2) | C24—C25—Fe3—C26 | 119.8 (3) |
| C2—C1—Fe1—C7 | −118.1 (2) | C25—C21—Fe3—C23 | −81.0 (3) |
| C26—C1—Fe1—C7 | −1.4 (4) | C22—C21—Fe3—C23 | 37.2 (3) |
| C2—C1—Fe1—C5 | 118.9 (3) | C16—C21—Fe3—C23 | 154.5 (5) |
| C26—C1—Fe1—C5 | −124.4 (5) | C25—C21—Fe3—C24 | −37.3 (2) |
| C5—C1—Fe1—C6 | 79.6 (3) | C22—C21—Fe3—C24 | 80.9 (3) |
| C2—C1—Fe1—C6 | −161.5 (2) | C16—C21—Fe3—C24 | −161.8 (5) |
| C26—C1—Fe1—C6 | −44.8 (5) | C25—C21—Fe3—C28 | 170.7 (2) |
| C7—C6—Fe1—C9 | −81.1 (3) | C22—C21—Fe3—C28 | −71.1 (3) |
| C10—C6—Fe1—C9 | 37.0 (3) | C16—C21—Fe3—C28 | 46.2 (5) |
| C11—C6—Fe1—C9 | 154.8 (4) | C25—C21—Fe3—C30 | 38.2 (6) |
| C7—C6—Fe1—C3 | −151.6 (4) | C22—C21—Fe3—C30 | 156.4 (4) |
| C10—C6—Fe1—C3 | −33.5 (5) | C16—C21—Fe3—C30 | −86.3 (6) |
| C11—C6—Fe1—C3 | 84.3 (5) | C25—C21—Fe3—C29 | −146.5 (5) |
| C7—C6—Fe1—C8 | −37.2 (2) | C22—C21—Fe3—C29 | −28.3 (6) |
| C10—C6—Fe1—C8 | 80.9 (3) | C16—C21—Fe3—C29 | 88.9 (6) |
| C11—C6—Fe1—C8 | −161.3 (4) | C25—C21—Fe3—C22 | −118.2 (4) |
| C7—C6—Fe1—C10 | −118.1 (3) | C16—C21—Fe3—C22 | 117.3 (5) |
| C11—C6—Fe1—C10 | 117.8 (5) | C25—C21—Fe3—C27 | 126.3 (2) |
| C7—C6—Fe1—C4 | 167.4 (2) | C22—C21—Fe3—C27 | −115.5 (3) |
| C10—C6—Fe1—C4 | −74.5 (3) | C16—C21—Fe3—C27 | 1.8 (4) |
| C11—C6—Fe1—C4 | 43.3 (4) | C22—C21—Fe3—C25 | 118.2 (4) |
| C7—C6—Fe1—C2 | 36.9 (6) | C16—C21—Fe3—C25 | −124.5 (5) |
| C10—C6—Fe1—C2 | 155.0 (5) | C25—C21—Fe3—C26 | 82.9 (3) |
| C11—C6—Fe1—C2 | −87.2 (7) | C22—C21—Fe3—C26 | −158.9 (3) |
| C10—C6—Fe1—C7 | 118.1 (3) | C16—C21—Fe3—C26 | −41.6 (5) |
| C11—C6—Fe1—C7 | −124.1 (4) | C27—C26—Fe3—C23 | −145.1 (5) |
| C7—C6—Fe1—C5 | 123.4 (2) | C30—C26—Fe3—C23 | −25.6 (6) |
| C10—C6—Fe1—C5 | −118.5 (3) | C1—C26—Fe3—C23 | 91.4 (6) |
| C11—C6—Fe1—C5 | −0.7 (4) | C27—C26—Fe3—C24 | 170.5 (2) |
| C7—C6—Fe1—C1 | 80.3 (3) | C30—C26—Fe3—C24 | −70.0 (3) |
| C10—C6—Fe1—C1 | −161.6 (3) | C1—C26—Fe3—C24 | 47.0 (4) |
| C11—C6—Fe1—C1 | −43.8 (5) | C27—C26—Fe3—C28 | −37.5 (2) |
| C18—C19—Fe2—C13 | −120.8 (3) | C30—C26—Fe3—C28 | 82.0 (3) |
| C20—C19—Fe2—C13 | 120.2 (3) | C1—C26—Fe3—C28 | −161.1 (4) |
| C18—C19—Fe2—C14 | −160.3 (3) | C27—C26—Fe3—C30 | −119.5 (3) |
| C20—C19—Fe2—C14 | 80.7 (3) | C1—C26—Fe3—C30 | 117.0 (5) |
| C18—C19—Fe2—C20 | 119.0 (4) | C27—C26—Fe3—C29 | −81.0 (3) |
| C18—C19—Fe2—C12 | −81.5 (3) | C30—C26—Fe3—C29 | 38.4 (3) |
| C20—C19—Fe2—C12 | 159.5 (2) | C1—C26—Fe3—C29 | 155.4 (5) |

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| C20—C19—Fe2—C18 | −119.0 (4) | C27—C26—Fe3—C22 | 37.6 (6) |
| C18—C19—Fe2—C15 | 178.5 (3) | C30—C26—Fe3—C22 | 157.0 (5) |
| C20—C19—Fe2—C15 | 59.5 (5) | C1—C26—Fe3—C22 | −86.0 (6) |
| C18—C19—Fe2—C17 | 37.8 (2) | C30—C26—Fe3—C27 | 119.5 (3) |
| C20—C19—Fe2—C17 | −81.2 (3) | C1—C26—Fe3—C27 | −123.6 (5) |
| C18—C19—Fe2—C11 | −62.1 (5) | C27—C26—Fe3—C25 | 126.0 (2) |
| C20—C19—Fe2—C11 | 178.9 (4) | C30—C26—Fe3—C25 | −114.6 (3) |
| C18—C19—Fe2—C16 | 81.1 (3) | C1—C26—Fe3—C25 | 2.4 (4) |
| C20—C19—Fe2—C16 | −37.9 (2) | C27—C26—Fe3—C21 | 82.0 (3) |
| C14—C13—Fe2—C19 | −118.9 (3) | C30—C26—Fe3—C21 | −158.6 (3) |
| C12—C13—Fe2—C19 | 121.8 (3) | C1—C26—Fe3—C21 | −41.6 (5) |
| C12—C13—Fe2—C14 | −119.3 (4) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg4 are the centroids of the C1–C5 and C16–C20 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C30—H30···*Cg*1$^{i}$ | 0.98 | 2.89 | 3.668 (5) | 137 |
| C28—H28···*Cg*4$^{ii}$ | 0.98 | 2.70 | 3.601 (6) | 153 |

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