

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(*R,R*)-*N,N'*-Bis(ferrocenylmethyl)cyclohexane-1,2-diamine

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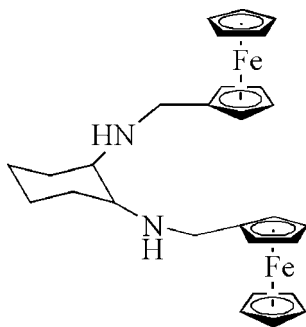
Received 22 June 2009; accepted 29 June 2009

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å;
 R factor = 0.042; wR factor = 0.087; data-to-parameter ratio = 18.9.

In the structure of the title compound, $[\text{Fe}_2(\text{C}_5\text{H}_5)_2(\text{C}_{18}\text{H}_{24}\text{N}_2)]$, the cyclohexane ring has a chair configuration and the two ferrocenemethylamino groups are bonded to it equatorially, as expected. The configuration of the two ferrocene nuclei may be due to intramolecular $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonding involving the two NH groups.

Related literature

For the applications of ferrocene derivatives, see: Yang *et al.* (2002); Roberto *et al.* (2000); Beer (1998). For the crystal structures of related compounds, see: Hess *et al.* (1999); Base *et al.* (2002). For the synthetic strategy, see: Cho *et al.* (1999); Sutcliffe (2002).



Experimental

Crystal data

$[\text{Fe}_2(\text{C}_5\text{H}_5)_2(\text{C}_{18}\text{H}_{24}\text{N}_2)]$
 $M_r = 510.27$
Monoclinic, $P2_1$
 $a = 5.9384$ (7) Å
 $b = 10.5310$ (11) Å
 $c = 19.173$ (3) Å
 $\beta = 90.989$ (10)°

$V = 1198.9$ (3) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 1.23$ mm⁻¹
 $T = 293$ K
0.15 × 0.12 × 0.10 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan
(*CrystalClear*; Rigaku, 2005)
 $T_{\text{min}} = 0.856$, $T_{\text{max}} = 1.000$
(expected range = 0.757–0.884)

12081 measured reflections
5474 independent reflections
4717 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.087$
 $S = 1.06$
5474 reflections
290 parameters
1 restraint

H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.27$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.45$ e Å⁻³
Absolute structure: Flack (1983),
2571 Friedel pairs
Flack parameter: 0.035 (19)

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---------------------------------------|--------------|--------------------|-------------|----------------------|
| $\text{N1}-\text{H1A}\cdots\text{N2}$ | 0.90 | 2.36 | 2.848 (4) | 114 |

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by a start-up grant from Southeast University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2124).

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supporting information

Acta Cryst. (2009). E65, m874 [doi:10.1107/S1600536809025057]

(*R,R*)-*N,N'*-Bis(ferrocenylmethyl)cyclohexane-1,2-diamine**YingChun Wang****S1. Comment**

The chemistry of ferrocene has received much attention as both ferrocene and its derivatives have applications in many fields. For example, ferrocene has been employed as a marker for the electrochemical detection of amino acids in selective anion sensors (Beer *et al.*, 1998). It also has applications in catalysis (Yang *et al.*, 2002), non-linear optical (NLO) materials (Roberto *et al.*, 2000) and medicinal materials. As part of our continuing studies on new ferrocene compounds, we report herein on the crystal structure of the title compound,

R,R—*N*¹,*N*²-Cyclohexane-1,2-bis((ferrocenylmethylene)amine, (I).

The molecular structure of the title compound is illustrated in Fig. 1. It consists of (*1R,2R*)-cyclohexane-1,2-diamine units, in which the hydrogen atoms of the two amine groups have been substituted by ferrocenylmethyl units. The cyclohexane ring has a chair conformation and the two ferrocenemethylamino groups are equatorially bonded to it, with torsion angles C1—C11—N1—C12 and C19—C18—N2—C17 being 178.4 (3) and 168.3 (3)°, respectively. The bond lengths and angles and the conformation of the ferrocenyl group, are similar to those observed in other ferrocenemethylamino derivatives (Hess *et al.*, 1999; Base *et al.*, 2002). The Cp ring planes (C6—C10 and C19—C23), are inclined to one another by 48.84 (15)°. The intramolecular Fe—Fe distance is 7.6054 (11) Å, while the nearest intermolecular Fe—Fe separation is 5.9384 (7) Å. The orientation of the two ferrocene nuclei is probably due to the presence of the intramolecular N1—H1...N22 hydrogen bond (Table 1).

The crystal packing of the title compound is illustrated in Fig. 2.

S2. Experimental

The title compound was synthesized by reducing the corresponding Schiff base (*R,R*—N1,N2-Cyclohexane-1,2-bis-((ferrocenylmethylene)) (5 mmol) (Cho *et al.*, 1999), with sodium borohydride (40 mmol) in methanol, in an ice bath. 40 ml NaOH solution (1 mol.L⁻¹) was added and the mixture was stirred at rt for an 1 h (Sutcliffe *et al.*, 2002)). The mixture was extracted with CHCl₃ and the solvent removed under vacuum. The crude product was purified by recrystallization from acetone. Red crystals, suitable for X-ray diffraction analysis, were obtained by slow evaporation of a methanol solution after 3 days.

S3. Refinement

The H-atoms were included in calculated positions and treated as riding atoms: N—H = 0.86 Å, C—H = 0.93 - 0.97 Å, with U_{iso}(H) = 1.2U_{eq}(parent N- or C-atom).

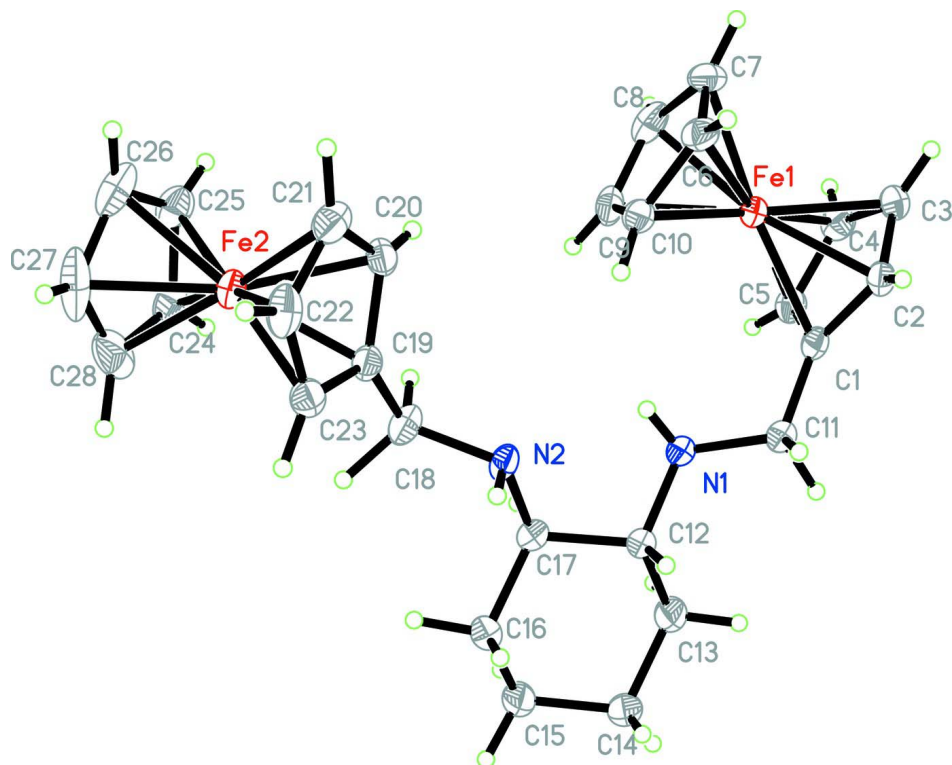
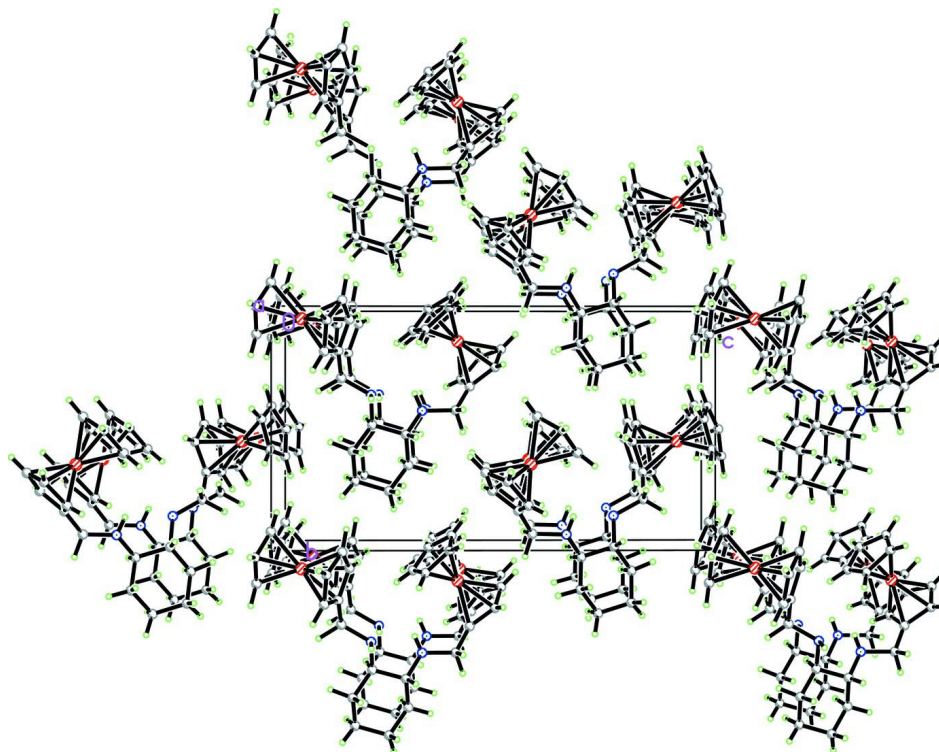


Figure 1

A view of the molecular structure of the title compound, with the displacement ellipsoids were drawn at the 30% probability level.

**Figure 2**

A crystal packing diagram of the title compound, viewed along the *a* axis.

(*R,R*)-*N,N'*-Bis(ferrocenylmethyl)cyclohexane-1,2-diamine

Crystal data

[Fe₂(C₅H₅)₂(C₁₈H₂₄N₂)]

M_r = 510.27

Monoclinic, *P2*₁

Hall symbol: P 2yb

a = 5.9384 (7) Å

b = 10.5310 (11) Å

c = 19.173 (3) Å

β = 90.989 (10)°

V = 1198.9 (3) Å³

Z = 2

F(000) = 536

D_x = 1.413 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 3140 reflections

θ = 3.2–27.5°

μ = 1.23 mm⁻¹

T = 293 K

Block, yellow

0.15 × 0.12 × 0.10 mm

Data collection

Rigaku SCXmini
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 13.6612 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrystalClear*; Rigaku, 2005)

T_{min} = 0.856, *T_{max}* = 1.000

12081 measured reflections

5474 independent reflections

4717 reflections with *I* > 2σ(*I*)

R_{int} = 0.044

θ_{\max} = 27.5°, θ_{\min} = 3.2°

h = -7→7

k = -13→13

l = -24→24

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.042$ $wR(F^2) = 0.087$ $S = 1.06$

5474 reflections

290 parameters

1 restraint

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0266P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.005$ $\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.45 \text{ e } \text{\AA}^{-3}$ Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0039 (6)

Absolute structure: Flack (1983), 2567 Friedel
pairs

Absolute structure parameter: 0.035 (19)

*Special details***Geometry.** Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles**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 (\AA^2)*

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|-------------|--------------|----------------------------------|
| Fe1 | -0.30550 (8) | 0.14014 (4) | 0.41771 (2) | 0.0319 (2) |
| Fe2 | 0.31701 (8) | 0.05780 (4) | 0.07731 (2) | 0.0359 (2) |
| N1 | -0.1496 (5) | 0.4290 (3) | 0.33760 (15) | 0.0420 (10) |
| N2 | 0.1430 (5) | 0.3628 (3) | 0.22723 (15) | 0.0424 (10) |
| C1 | -0.2745 (6) | 0.3278 (3) | 0.44519 (18) | 0.0346 (10) |
| C2 | -0.2197 (6) | 0.2484 (3) | 0.50262 (18) | 0.0379 (11) |
| C3 | -0.4105 (7) | 0.1713 (4) | 0.5177 (2) | 0.0439 (12) |
| C4 | -0.5809 (6) | 0.2026 (4) | 0.4685 (2) | 0.0455 (11) |
| C5 | -0.4994 (6) | 0.2994 (3) | 0.42391 (19) | 0.0392 (11) |
| C6 | -0.0664 (6) | 0.0033 (3) | 0.40032 (19) | 0.0433 (11) |
| C7 | -0.2839 (6) | -0.0511 (3) | 0.4033 (2) | 0.0482 (11) |
| C8 | -0.4153 (7) | 0.0049 (4) | 0.3496 (2) | 0.0527 (14) |
| C9 | -0.2840 (7) | 0.0948 (4) | 0.3144 (2) | 0.0484 (14) |
| C10 | -0.0653 (6) | 0.0945 (3) | 0.34622 (18) | 0.0403 (11) |
| C11 | -0.1262 (6) | 0.4267 (3) | 0.41367 (18) | 0.0421 (11) |
| C12 | -0.0144 (7) | 0.5256 (3) | 0.30284 (19) | 0.0412 (11) |
| C13 | -0.1359 (8) | 0.6533 (4) | 0.3064 (2) | 0.0589 (14) |
| C14 | -0.0159 (9) | 0.7556 (4) | 0.2652 (2) | 0.069 (2) |
| C15 | 0.0105 (10) | 0.7148 (4) | 0.1895 (2) | 0.0685 (16) |
| C16 | 0.1400 (8) | 0.5900 (4) | 0.1867 (2) | 0.0578 (14) |
| C17 | 0.0245 (7) | 0.4849 (4) | 0.2277 (2) | 0.0427 (11) |
| C18 | 0.1208 (6) | 0.2940 (4) | 0.16031 (19) | 0.0484 (12) |

| | | | | |
|------|------------|-------------|--------------|-------------|
| C19 | 0.2803 (6) | 0.1851 (3) | 0.15736 (18) | 0.0363 (11) |
| C20 | 0.2432 (6) | 0.0588 (4) | 0.18120 (17) | 0.0405 (11) |
| C21 | 0.4394 (7) | -0.0130 (4) | 0.1695 (2) | 0.0498 (12) |
| C22 | 0.5983 (6) | 0.0673 (4) | 0.13930 (18) | 0.0508 (13) |
| C23 | 0.5017 (6) | 0.1894 (4) | 0.13173 (19) | 0.0418 (11) |
| C24 | 0.0702 (7) | 0.0889 (4) | 0.0051 (2) | 0.0582 (14) |
| C25 | 0.0701 (7) | -0.0383 (4) | 0.0239 (2) | 0.0531 (16) |
| C26 | 0.2822 (8) | -0.0894 (5) | 0.0087 (2) | 0.0665 (17) |
| C27 | 0.4131 (7) | 0.0072 (7) | -0.0203 (2) | 0.080 (2) |
| C28 | 0.2810 (9) | 0.1171 (6) | -0.0231 (2) | 0.077 (2) |
| H1A | -0.10720 | 0.35250 | 0.32140 | 0.0500* |
| H2A | -0.07450 | 0.24620 | 0.52770 | 0.0450* |
| H2C | 0.29010 | 0.37760 | 0.23580 | 0.0510* |
| H3A | -0.42060 | 0.10780 | 0.55490 | 0.0530* |
| H4A | -0.73120 | 0.16430 | 0.46570 | 0.0550* |
| H5A | -0.58320 | 0.33930 | 0.38530 | 0.0470* |
| H6A | 0.06100 | -0.01700 | 0.43150 | 0.0520* |
| H7A | -0.33290 | -0.11700 | 0.43580 | 0.0580* |
| H8A | -0.57340 | -0.01500 | 0.33880 | 0.0640* |
| H9A | -0.33370 | 0.14780 | 0.27500 | 0.0580* |
| H10A | 0.06260 | 0.14750 | 0.33290 | 0.0480* |
| H11A | -0.16520 | 0.50940 | 0.43220 | 0.0500* |
| H11B | 0.02950 | 0.40940 | 0.42660 | 0.0500* |
| H12A | 0.13150 | 0.53290 | 0.32720 | 0.0490* |
| H13A | -0.28810 | 0.64350 | 0.28800 | 0.0710* |
| H13B | -0.14530 | 0.67960 | 0.35470 | 0.0710* |
| H14A | 0.13140 | 0.77130 | 0.28610 | 0.0830* |
| H14B | -0.10150 | 0.83390 | 0.26700 | 0.0830* |
| H15A | -0.13680 | 0.70420 | 0.16760 | 0.0820* |
| H15B | 0.09100 | 0.77980 | 0.16410 | 0.0820* |
| H16A | 0.29080 | 0.60290 | 0.20570 | 0.0690* |
| H16B | 0.15340 | 0.56370 | 0.13840 | 0.0690* |
| H17A | -0.12390 | 0.47120 | 0.20580 | 0.0510* |
| H18A | 0.15040 | 0.35190 | 0.12220 | 0.0580* |
| H18B | -0.03220 | 0.26300 | 0.15460 | 0.0580* |
| H20A | 0.10410 | 0.02690 | 0.20170 | 0.0480* |
| H21A | 0.46100 | -0.10290 | 0.18080 | 0.0600* |
| H22A | 0.75080 | 0.04300 | 0.12580 | 0.0610* |
| H23A | 0.57550 | 0.26400 | 0.11190 | 0.0500* |
| H24A | -0.05610 | 0.14810 | 0.00960 | 0.0700* |
| H25A | -0.05550 | -0.08430 | 0.04460 | 0.0640* |
| H26A | 0.33020 | -0.17720 | 0.01690 | 0.0800* |
| H27A | 0.56820 | -0.00110 | -0.03640 | 0.0960* |
| H28A | 0.32780 | 0.19970 | -0.04130 | 0.0920* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Fe1 | 0.0361 (3) | 0.0313 (3) | 0.0283 (3) | 0.0006 (2) | 0.0029 (2) | -0.0026 (2) |
| Fe2 | 0.0349 (3) | 0.0429 (3) | 0.0298 (3) | 0.0027 (3) | -0.0002 (2) | -0.0080 (2) |
| N1 | 0.063 (2) | 0.0298 (15) | 0.0337 (17) | -0.0066 (14) | 0.0129 (14) | -0.0055 (13) |
| N2 | 0.0559 (19) | 0.0376 (16) | 0.0339 (16) | 0.0043 (14) | 0.0064 (14) | -0.0109 (13) |
| C1 | 0.0415 (18) | 0.0341 (18) | 0.0285 (18) | 0.0034 (15) | 0.0058 (14) | -0.0078 (14) |
| C2 | 0.046 (2) | 0.041 (2) | 0.0267 (18) | -0.0007 (17) | 0.0006 (15) | -0.0047 (14) |
| C3 | 0.057 (2) | 0.043 (2) | 0.032 (2) | -0.0020 (19) | 0.0139 (17) | -0.0036 (16) |
| C4 | 0.0378 (18) | 0.049 (2) | 0.050 (2) | -0.0018 (17) | 0.0097 (17) | -0.0082 (18) |
| C5 | 0.0350 (17) | 0.0418 (19) | 0.041 (2) | 0.0060 (15) | 0.0048 (15) | -0.0042 (16) |
| C6 | 0.049 (2) | 0.0328 (17) | 0.048 (2) | 0.0058 (16) | 0.0003 (17) | -0.0036 (16) |
| C7 | 0.061 (2) | 0.0311 (19) | 0.053 (2) | -0.0061 (17) | 0.013 (2) | 0.0020 (17) |
| C8 | 0.046 (2) | 0.054 (2) | 0.058 (3) | -0.004 (2) | -0.002 (2) | -0.025 (2) |
| C9 | 0.066 (3) | 0.050 (2) | 0.0290 (19) | 0.016 (2) | -0.0021 (17) | -0.0073 (17) |
| C10 | 0.0485 (19) | 0.0336 (17) | 0.0393 (19) | 0.0017 (16) | 0.0127 (16) | -0.0028 (15) |
| C11 | 0.053 (2) | 0.0363 (18) | 0.037 (2) | -0.0050 (17) | 0.0055 (16) | -0.0060 (15) |
| C12 | 0.060 (2) | 0.0322 (19) | 0.0317 (19) | -0.0089 (17) | 0.0062 (17) | -0.0033 (15) |
| C13 | 0.096 (3) | 0.039 (2) | 0.042 (2) | 0.005 (2) | 0.014 (2) | -0.001 (2) |
| C14 | 0.130 (5) | 0.030 (2) | 0.047 (3) | -0.006 (3) | 0.015 (3) | -0.0015 (19) |
| C15 | 0.130 (4) | 0.035 (2) | 0.041 (2) | -0.003 (3) | 0.019 (3) | 0.003 (2) |
| C16 | 0.089 (3) | 0.043 (2) | 0.042 (2) | -0.010 (2) | 0.021 (2) | 0.0010 (18) |
| C17 | 0.057 (2) | 0.0331 (19) | 0.038 (2) | -0.0017 (18) | 0.0055 (17) | -0.0046 (16) |
| C18 | 0.057 (2) | 0.047 (2) | 0.041 (2) | 0.0072 (19) | -0.0060 (19) | -0.0137 (18) |
| C19 | 0.0371 (18) | 0.0406 (19) | 0.0314 (19) | -0.0026 (16) | 0.0031 (15) | -0.0064 (15) |
| C20 | 0.0461 (18) | 0.046 (2) | 0.0297 (17) | -0.0076 (19) | 0.0055 (14) | -0.0043 (17) |
| C21 | 0.061 (2) | 0.044 (2) | 0.044 (2) | 0.013 (2) | -0.0119 (19) | -0.0073 (18) |
| C22 | 0.0384 (18) | 0.075 (3) | 0.039 (2) | 0.011 (2) | -0.0018 (15) | -0.011 (2) |
| C23 | 0.0385 (18) | 0.050 (2) | 0.037 (2) | -0.0132 (17) | 0.0007 (15) | -0.0054 (16) |
| C24 | 0.061 (2) | 0.064 (3) | 0.049 (2) | 0.014 (2) | -0.019 (2) | -0.012 (2) |
| C25 | 0.049 (2) | 0.057 (3) | 0.053 (3) | -0.006 (2) | -0.0048 (18) | -0.015 (2) |
| C26 | 0.069 (3) | 0.069 (3) | 0.061 (3) | 0.020 (3) | -0.012 (3) | -0.038 (3) |
| C27 | 0.042 (2) | 0.157 (6) | 0.041 (3) | -0.008 (3) | 0.008 (2) | -0.037 (3) |
| C28 | 0.102 (4) | 0.097 (4) | 0.030 (2) | -0.041 (4) | -0.013 (2) | 0.010 (2) |

Geometric parameters (Å, °)

| | | | |
|---------|-----------|---------|-----------|
| Fe1—C1 | 2.053 (3) | C18—C19 | 1.489 (5) |
| Fe1—C2 | 2.045 (3) | C19—C20 | 1.425 (5) |
| Fe1—C3 | 2.053 (4) | C19—C23 | 1.412 (5) |
| Fe1—C4 | 2.028 (4) | C20—C21 | 1.410 (6) |
| Fe1—C5 | 2.039 (3) | C21—C22 | 1.400 (6) |
| Fe1—C6 | 2.054 (3) | C22—C23 | 1.414 (6) |
| Fe1—C7 | 2.037 (3) | C24—C28 | 1.404 (7) |
| Fe1—C8 | 2.032 (4) | C24—C25 | 1.387 (6) |
| Fe1—C9 | 2.044 (4) | C25—C26 | 1.405 (6) |
| Fe1—C10 | 2.052 (4) | C26—C27 | 1.401 (8) |

| | | | |
|------------|-------------|-------------|------------|
| Fe2—C19 | 2.052 (3) | C27—C28 | 1.399 (9) |
| Fe2—C20 | 2.047 (3) | C2—H2A | 0.9800 |
| Fe2—C21 | 2.041 (4) | C3—H3A | 0.9800 |
| Fe2—C22 | 2.036 (4) | C4—H4A | 0.9800 |
| Fe2—C23 | 2.043 (4) | C5—H5A | 0.9800 |
| Fe2—C24 | 2.025 (4) | C6—H6A | 0.9800 |
| Fe2—C25 | 2.042 (4) | C7—H7A | 0.9800 |
| Fe2—C26 | 2.041 (5) | C8—H8A | 0.9800 |
| Fe2—C27 | 2.037 (4) | C9—H9A | 0.9800 |
| Fe2—C28 | 2.032 (4) | C10—H10A | 0.9800 |
| N1—C11 | 1.463 (4) | C11—H11A | 0.9700 |
| N1—C12 | 1.464 (5) | C11—H11B | 0.9700 |
| N2—C17 | 1.466 (5) | C12—H12A | 0.9800 |
| N2—C18 | 1.477 (5) | C13—H13A | 0.9700 |
| N1—H1A | 0.9000 | C13—H13B | 0.9700 |
| N2—H2C | 0.9000 | C14—H14A | 0.9700 |
| C1—C5 | 1.422 (5) | C14—H14B | 0.9700 |
| C1—C11 | 1.498 (5) | C15—H15A | 0.9700 |
| C1—C2 | 1.416 (5) | C15—H15B | 0.9700 |
| C2—C3 | 1.428 (5) | C16—H16A | 0.9700 |
| C3—C4 | 1.411 (5) | C16—H16B | 0.9700 |
| C4—C5 | 1.421 (5) | C17—H17A | 0.9800 |
| C6—C10 | 1.414 (5) | C18—H18A | 0.9700 |
| C6—C7 | 1.415 (5) | C18—H18B | 0.9700 |
| C7—C8 | 1.410 (5) | C20—H20A | 0.9800 |
| C8—C9 | 1.406 (6) | C21—H21A | 0.9800 |
| C9—C10 | 1.425 (5) | C22—H22A | 0.9800 |
| C12—C17 | 1.525 (5) | C23—H23A | 0.9800 |
| C12—C13 | 1.528 (6) | C24—H24A | 0.9800 |
| C13—C14 | 1.521 (6) | C25—H25A | 0.9800 |
| C14—C15 | 1.524 (6) | C26—H26A | 0.9800 |
| C15—C16 | 1.524 (6) | C27—H27A | 0.9800 |
| C16—C17 | 1.527 (6) | C28—H28A | 0.9800 |
| C1—Fe1—C2 | 40.43 (13) | N1—C12—C17 | 109.2 (3) |
| C1—Fe1—C3 | 68.51 (15) | C12—C13—C14 | 112.0 (4) |
| C1—Fe1—C4 | 68.52 (15) | C13—C14—C15 | 110.6 (4) |
| C1—Fe1—C5 | 40.66 (14) | C14—C15—C16 | 109.7 (3) |
| C1—Fe1—C6 | 131.14 (14) | C15—C16—C17 | 112.1 (4) |
| C1—Fe1—C7 | 168.82 (15) | N2—C17—C12 | 109.5 (3) |
| C1—Fe1—C8 | 150.00 (15) | N2—C17—C16 | 114.4 (3) |
| C1—Fe1—C9 | 117.83 (15) | C12—C17—C16 | 111.1 (3) |
| C1—Fe1—C10 | 109.67 (13) | N2—C18—C19 | 111.3 (3) |
| C2—Fe1—C3 | 40.78 (15) | Fe2—C19—C18 | 127.4 (3) |
| C2—Fe1—C4 | 68.20 (15) | Fe2—C19—C20 | 69.46 (19) |
| C2—Fe1—C5 | 68.17 (14) | C20—C19—C23 | 107.0 (3) |
| C2—Fe1—C6 | 110.91 (14) | C18—C19—C23 | 125.8 (3) |
| C2—Fe1—C7 | 130.07 (14) | Fe2—C19—C23 | 69.5 (2) |

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| C2—Fe1—C8 | 167.21 (15) | C18—C19—C20 | 127.2 (3) |
| C2—Fe1—C9 | 152.01 (15) | Fe2—C20—C21 | 69.6 (2) |
| C2—Fe1—C10 | 119.72 (14) | C19—C20—C21 | 108.5 (3) |
| C3—Fe1—C4 | 40.44 (16) | Fe2—C20—C19 | 69.86 (19) |
| C3—Fe1—C5 | 68.48 (16) | Fe2—C21—C20 | 70.1 (2) |
| C3—Fe1—C6 | 119.06 (16) | Fe2—C21—C22 | 69.7 (2) |
| C3—Fe1—C7 | 107.79 (16) | C20—C21—C22 | 107.9 (4) |
| C3—Fe1—C8 | 127.81 (16) | Fe2—C22—C21 | 70.1 (2) |
| C3—Fe1—C9 | 165.40 (17) | Fe2—C22—C23 | 70.0 (2) |
| C3—Fe1—C10 | 152.51 (15) | C21—C22—C23 | 108.5 (3) |
| C4—Fe1—C5 | 40.90 (15) | Fe2—C23—C22 | 69.4 (2) |
| C4—Fe1—C6 | 150.58 (15) | C19—C23—C22 | 108.3 (3) |
| C4—Fe1—C7 | 116.05 (16) | Fe2—C23—C19 | 70.2 (2) |
| C4—Fe1—C8 | 106.47 (16) | C25—C24—C28 | 108.0 (4) |
| C4—Fe1—C9 | 127.28 (16) | Fe2—C24—C25 | 70.7 (2) |
| C4—Fe1—C10 | 166.52 (15) | Fe2—C24—C28 | 70.0 (2) |
| C5—Fe1—C6 | 168.25 (14) | Fe2—C25—C26 | 69.8 (3) |
| C5—Fe1—C7 | 149.10 (14) | C24—C25—C26 | 108.2 (4) |
| C5—Fe1—C8 | 116.02 (16) | Fe2—C25—C24 | 69.4 (2) |
| C5—Fe1—C9 | 107.07 (16) | Fe2—C26—C25 | 69.9 (3) |
| C5—Fe1—C10 | 129.14 (14) | Fe2—C26—C27 | 69.7 (3) |
| C6—Fe1—C7 | 40.46 (14) | C25—C26—C27 | 108.0 (4) |
| C6—Fe1—C8 | 67.61 (15) | Fe2—C27—C26 | 70.1 (2) |
| C6—Fe1—C9 | 67.91 (16) | Fe2—C27—C28 | 69.7 (3) |
| C6—Fe1—C10 | 40.27 (14) | C26—C27—C28 | 107.5 (4) |
| C7—Fe1—C8 | 40.56 (16) | Fe2—C28—C27 | 70.1 (3) |
| C7—Fe1—C9 | 68.44 (16) | C24—C28—C27 | 108.3 (5) |
| C7—Fe1—C10 | 68.39 (14) | Fe2—C28—C24 | 69.5 (2) |
| C8—Fe1—C9 | 40.37 (16) | Fe1—C2—H2A | 126.00 |
| C8—Fe1—C10 | 68.02 (15) | C1—C2—H2A | 126.00 |
| C9—Fe1—C10 | 40.73 (15) | C3—C2—H2A | 126.00 |
| C19—Fe2—C20 | 40.68 (15) | Fe1—C3—H3A | 126.00 |
| C19—Fe2—C21 | 68.39 (15) | C2—C3—H3A | 126.00 |
| C19—Fe2—C22 | 68.16 (15) | C4—C3—H3A | 126.00 |
| C19—Fe2—C23 | 40.35 (14) | Fe1—C4—H4A | 126.00 |
| C19—Fe2—C24 | 108.70 (15) | C3—C4—H4A | 126.00 |
| C19—Fe2—C25 | 127.88 (15) | C5—C4—H4A | 126.00 |
| C19—Fe2—C26 | 165.27 (16) | Fe1—C5—H5A | 126.00 |
| C19—Fe2—C27 | 153.3 (2) | C1—C5—H5A | 126.00 |
| C19—Fe2—C28 | 119.8 (2) | C4—C5—H5A | 126.00 |
| C20—Fe2—C21 | 40.36 (16) | Fe1—C6—H6A | 126.00 |
| C20—Fe2—C22 | 67.60 (14) | C7—C6—H6A | 126.00 |
| C20—Fe2—C23 | 67.76 (15) | C10—C6—H6A | 126.00 |
| C20—Fe2—C24 | 119.99 (15) | Fe1—C7—H7A | 126.00 |
| C20—Fe2—C25 | 109.06 (15) | C6—C7—H7A | 126.00 |
| C20—Fe2—C26 | 127.59 (17) | C8—C7—H7A | 126.00 |
| C20—Fe2—C27 | 164.5 (2) | Fe1—C8—H8A | 126.00 |
| C20—Fe2—C28 | 154.1 (2) | C7—C8—H8A | 125.00 |

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| C21—Fe2—C22 | 40.17 (16) | C9—C8—H8A | 125.00 |
| C21—Fe2—C23 | 68.00 (16) | Fe1—C9—H9A | 126.00 |
| C21—Fe2—C24 | 153.37 (17) | C8—C9—H9A | 126.00 |
| C21—Fe2—C25 | 119.68 (16) | C10—C9—H9A | 126.00 |
| C21—Fe2—C26 | 108.14 (17) | Fe1—C10—H10A | 126.00 |
| C21—Fe2—C27 | 126.8 (2) | C6—C10—H10A | 126.00 |
| C21—Fe2—C28 | 164.40 (19) | C9—C10—H10A | 126.00 |
| C22—Fe2—C23 | 40.58 (16) | N1—C11—H11A | 109.00 |
| C22—Fe2—C24 | 165.45 (17) | N1—C11—H11B | 109.00 |
| C22—Fe2—C25 | 153.11 (17) | C1—C11—H11A | 109.00 |
| C22—Fe2—C26 | 119.11 (18) | C1—C11—H11B | 109.00 |
| C22—Fe2—C27 | 108.01 (15) | H11A—C11—H11B | 108.00 |
| C22—Fe2—C28 | 127.59 (19) | N1—C12—H12A | 109.00 |
| C23—Fe2—C24 | 127.97 (16) | C13—C12—H12A | 109.00 |
| C23—Fe2—C25 | 165.20 (16) | C17—C12—H12A | 109.00 |
| C23—Fe2—C26 | 153.11 (17) | C12—C13—H13A | 109.00 |
| C23—Fe2—C27 | 119.36 (19) | C12—C13—H13B | 109.00 |
| C23—Fe2—C28 | 108.8 (2) | C14—C13—H13A | 109.00 |
| C24—Fe2—C25 | 39.88 (17) | C14—C13—H13B | 109.00 |
| C24—Fe2—C26 | 67.56 (18) | H13A—C13—H13B | 108.00 |
| C24—Fe2—C27 | 67.98 (17) | C13—C14—H14A | 109.00 |
| C24—Fe2—C28 | 40.49 (19) | C13—C14—H14B | 109.00 |
| C25—Fe2—C26 | 40.25 (18) | C15—C14—H14A | 110.00 |
| C25—Fe2—C27 | 67.65 (18) | C15—C14—H14B | 110.00 |
| C25—Fe2—C28 | 67.3 (2) | H14A—C14—H14B | 108.00 |
| C26—Fe2—C27 | 40.2 (2) | C14—C15—H15A | 110.00 |
| C26—Fe2—C28 | 67.4 (2) | C14—C15—H15B | 110.00 |
| C27—Fe2—C28 | 40.2 (2) | C16—C15—H15A | 110.00 |
| C11—N1—C12 | 115.0 (3) | C16—C15—H15B | 110.00 |
| C17—N2—C18 | 113.6 (3) | H15A—C15—H15B | 108.00 |
| C11—N1—H1A | 108.00 | C15—C16—H16A | 109.00 |
| C12—N1—H1A | 108.00 | C15—C16—H16B | 109.00 |
| C17—N2—H2C | 108.00 | C17—C16—H16A | 109.00 |
| C18—N2—H2C | 108.00 | C17—C16—H16B | 109.00 |
| C2—C1—C11 | 126.6 (3) | H16A—C16—H16B | 108.00 |
| C5—C1—C11 | 125.9 (3) | N2—C17—H17A | 107.00 |
| Fe1—C1—C5 | 69.15 (18) | C12—C17—H17A | 107.00 |
| Fe1—C1—C11 | 128.1 (2) | C16—C17—H17A | 107.00 |
| Fe1—C1—C2 | 69.48 (18) | N2—C18—H18A | 109.00 |
| C2—C1—C5 | 107.5 (3) | N2—C18—H18B | 109.00 |
| Fe1—C2—C1 | 70.09 (19) | C19—C18—H18A | 109.00 |
| Fe1—C2—C3 | 69.9 (2) | C19—C18—H18B | 109.00 |
| C1—C2—C3 | 108.7 (3) | H18A—C18—H18B | 108.00 |
| Fe1—C3—C2 | 69.3 (2) | Fe2—C20—H20A | 126.00 |
| Fe1—C3—C4 | 68.8 (2) | C19—C20—H20A | 126.00 |
| C2—C3—C4 | 107.1 (3) | C21—C20—H20A | 126.00 |
| Fe1—C4—C5 | 70.0 (2) | Fe2—C21—H21A | 126.00 |
| C3—C4—C5 | 108.8 (3) | C20—C21—H21A | 126.00 |

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| Fe1—C4—C3 | 70.7 (2) | C22—C21—H21A | 126.00 |
| C1—C5—C4 | 107.8 (3) | Fe2—C22—H22A | 126.00 |
| Fe1—C5—C4 | 69.1 (2) | C21—C22—H22A | 126.00 |
| Fe1—C5—C1 | 70.19 (19) | C23—C22—H22A | 126.00 |
| Fe1—C6—C7 | 69.12 (19) | Fe2—C23—H23A | 126.00 |
| C7—C6—C10 | 108.7 (3) | C19—C23—H23A | 126.00 |
| Fe1—C6—C10 | 69.79 (19) | C22—C23—H23A | 126.00 |
| Fe1—C7—C8 | 69.5 (2) | Fe2—C24—H24A | 126.00 |
| C6—C7—C8 | 107.2 (3) | C25—C24—H24A | 126.00 |
| Fe1—C7—C6 | 70.42 (19) | C28—C24—H24A | 126.00 |
| Fe1—C8—C7 | 69.9 (2) | Fe2—C25—H25A | 126.00 |
| Fe1—C8—C9 | 70.3 (2) | C24—C25—H25A | 126.00 |
| C7—C8—C9 | 109.1 (4) | C26—C25—H25A | 126.00 |
| Fe1—C9—C8 | 69.4 (2) | Fe2—C26—H26A | 126.00 |
| C8—C9—C10 | 107.6 (3) | C25—C26—H26A | 126.00 |
| Fe1—C9—C10 | 70.0 (2) | C27—C26—H26A | 126.00 |
| Fe1—C10—C6 | 69.9 (2) | Fe2—C27—H27A | 126.00 |
| Fe1—C10—C9 | 69.3 (2) | C26—C27—H27A | 126.00 |
| C6—C10—C9 | 107.5 (3) | C28—C27—H27A | 126.00 |
| N1—C11—C1 | 111.6 (3) | Fe2—C28—H28A | 126.00 |
| C13—C12—C17 | 111.7 (3) | C24—C28—H28A | 126.00 |
| N1—C12—C13 | 109.2 (3) | C27—C28—H28A | 126.00 |
| | | | |
| C2—Fe1—C1—C5 | -119.1 (3) | C26—Fe2—C21—C20 | -127.3 (3) |
| C2—Fe1—C1—C11 | 121.0 (4) | C26—Fe2—C21—C22 | 113.9 (3) |
| C3—Fe1—C1—C2 | 37.6 (2) | C27—Fe2—C21—C20 | -167.9 (3) |
| C3—Fe1—C1—C5 | -81.6 (2) | C27—Fe2—C21—C22 | 73.3 (3) |
| C3—Fe1—C1—C11 | 158.5 (4) | C19—Fe2—C22—C21 | 81.9 (2) |
| C4—Fe1—C1—C2 | 81.2 (2) | C19—Fe2—C22—C23 | -37.4 (2) |
| C4—Fe1—C1—C5 | -37.9 (2) | C20—Fe2—C22—C21 | 37.9 (2) |
| C4—Fe1—C1—C11 | -157.9 (3) | C20—Fe2—C22—C23 | -81.5 (2) |
| C5—Fe1—C1—C2 | 119.1 (3) | C21—Fe2—C22—C23 | -119.4 (3) |
| C5—Fe1—C1—C11 | -119.9 (4) | C23—Fe2—C22—C21 | 119.4 (3) |
| C6—Fe1—C1—C2 | -72.9 (3) | C25—Fe2—C22—C21 | -50.3 (4) |
| C6—Fe1—C1—C5 | 168.0 (2) | C25—Fe2—C22—C23 | -169.7 (3) |
| C6—Fe1—C1—C11 | 48.1 (4) | C26—Fe2—C22—C21 | -83.8 (3) |
| C8—Fe1—C1—C2 | 167.0 (3) | C26—Fe2—C22—C23 | 156.8 (2) |
| C8—Fe1—C1—C5 | 47.9 (4) | C27—Fe2—C22—C21 | -126.3 (3) |
| C8—Fe1—C1—C11 | -72.0 (5) | C27—Fe2—C22—C23 | 114.4 (3) |
| C9—Fe1—C1—C2 | -156.9 (2) | C28—Fe2—C22—C21 | -166.5 (3) |
| C9—Fe1—C1—C5 | 84.0 (2) | C28—Fe2—C22—C23 | 74.1 (3) |
| C9—Fe1—C1—C11 | -36.0 (4) | C19—Fe2—C23—C22 | 119.4 (3) |
| C10—Fe1—C1—C2 | -113.1 (2) | C20—Fe2—C23—C19 | -38.4 (2) |
| C10—Fe1—C1—C5 | 127.8 (2) | C20—Fe2—C23—C22 | 81.1 (2) |
| C10—Fe1—C1—C11 | 7.9 (3) | C21—Fe2—C23—C19 | -82.1 (2) |
| C1—Fe1—C2—C3 | 119.7 (3) | C21—Fe2—C23—C22 | 37.3 (2) |
| C3—Fe1—C2—C1 | -119.7 (3) | C22—Fe2—C23—C19 | -119.4 (3) |
| C4—Fe1—C2—C1 | -82.0 (2) | C24—Fe2—C23—C19 | 73.1 (3) |

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| C4—Fe1—C2—C3 | 37.7 (2) | C24—Fe2—C23—C22 | -167.5 (2) |
| C5—Fe1—C2—C1 | -37.8 (2) | C26—Fe2—C23—C19 | -169.0 (3) |
| C5—Fe1—C2—C3 | 81.9 (2) | C26—Fe2—C23—C22 | -49.6 (4) |
| C6—Fe1—C2—C1 | 129.6 (2) | C27—Fe2—C23—C19 | 157.0 (3) |
| C6—Fe1—C2—C3 | -110.7 (2) | C27—Fe2—C23—C22 | -83.6 (3) |
| C7—Fe1—C2—C1 | 171.6 (2) | C28—Fe2—C23—C19 | 114.2 (2) |
| C7—Fe1—C2—C3 | -68.7 (3) | C28—Fe2—C23—C22 | -126.4 (2) |
| C9—Fe1—C2—C1 | 47.6 (4) | C19—Fe2—C24—C25 | -127.3 (2) |
| C9—Fe1—C2—C3 | 167.3 (3) | C19—Fe2—C24—C28 | 114.3 (3) |
| C10—Fe1—C2—C1 | 85.9 (2) | C20—Fe2—C24—C25 | -84.1 (3) |
| C10—Fe1—C2—C3 | -154.4 (2) | C20—Fe2—C24—C28 | 157.5 (3) |
| C1—Fe1—C3—C2 | -37.3 (2) | C21—Fe2—C24—C25 | -48.4 (5) |
| C1—Fe1—C3—C4 | 81.7 (3) | C21—Fe2—C24—C28 | -166.8 (4) |
| C2—Fe1—C3—C4 | 118.9 (3) | C23—Fe2—C24—C25 | -168.1 (2) |
| C4—Fe1—C3—C2 | -118.9 (3) | C23—Fe2—C24—C28 | 73.5 (3) |
| C5—Fe1—C3—C2 | -81.1 (2) | C25—Fe2—C24—C28 | -118.4 (4) |
| C5—Fe1—C3—C4 | 37.8 (2) | C26—Fe2—C24—C25 | 37.5 (2) |
| C6—Fe1—C3—C2 | 88.9 (2) | C26—Fe2—C24—C28 | -80.9 (3) |
| C6—Fe1—C3—C4 | -152.2 (2) | C27—Fe2—C24—C25 | 81.0 (3) |
| C7—Fe1—C3—C2 | 131.5 (2) | C27—Fe2—C24—C28 | -37.4 (4) |
| C7—Fe1—C3—C4 | -109.5 (2) | C28—Fe2—C24—C25 | 118.4 (4) |
| C8—Fe1—C3—C2 | 172.0 (2) | C19—Fe2—C25—C24 | 72.7 (3) |
| C8—Fe1—C3—C4 | -69.1 (3) | C19—Fe2—C25—C26 | -167.8 (2) |
| C10—Fe1—C3—C2 | 54.3 (4) | C20—Fe2—C25—C24 | 114.3 (2) |
| C10—Fe1—C3—C4 | 173.2 (3) | C20—Fe2—C25—C26 | -126.2 (3) |
| C1—Fe1—C4—C3 | -81.7 (2) | C21—Fe2—C25—C24 | 157.3 (2) |
| C1—Fe1—C4—C5 | 37.7 (2) | C21—Fe2—C25—C26 | -83.2 (3) |
| C2—Fe1—C4—C3 | -38.0 (2) | C22—Fe2—C25—C24 | -167.9 (3) |
| C2—Fe1—C4—C5 | 81.4 (2) | C22—Fe2—C25—C26 | -48.3 (4) |
| C3—Fe1—C4—C5 | 119.4 (3) | C24—Fe2—C25—C26 | 119.5 (3) |
| C5—Fe1—C4—C3 | -119.4 (3) | C26—Fe2—C25—C24 | -119.5 (3) |
| C6—Fe1—C4—C3 | 56.2 (4) | C27—Fe2—C25—C24 | -82.0 (3) |
| C6—Fe1—C4—C5 | 175.6 (3) | C27—Fe2—C25—C26 | 37.6 (3) |
| C7—Fe1—C4—C3 | 87.2 (3) | C28—Fe2—C25—C24 | -38.3 (3) |
| C7—Fe1—C4—C5 | -153.4 (2) | C28—Fe2—C25—C26 | 81.3 (3) |
| C8—Fe1—C4—C3 | 129.7 (2) | C20—Fe2—C26—C25 | 74.2 (3) |
| C8—Fe1—C4—C5 | -110.9 (2) | C20—Fe2—C26—C27 | -166.7 (3) |
| C9—Fe1—C4—C3 | 169.0 (2) | C21—Fe2—C26—C25 | 114.8 (3) |
| C9—Fe1—C4—C5 | -71.6 (3) | C21—Fe2—C26—C27 | -126.1 (3) |
| C1—Fe1—C5—C4 | -119.1 (3) | C22—Fe2—C26—C25 | 157.2 (2) |
| C2—Fe1—C5—C1 | 37.6 (2) | C22—Fe2—C26—C27 | -83.6 (3) |
| C2—Fe1—C5—C4 | -81.5 (2) | C23—Fe2—C26—C25 | -168.2 (3) |
| C3—Fe1—C5—C1 | 81.7 (2) | C23—Fe2—C26—C27 | -49.1 (5) |
| C3—Fe1—C5—C4 | -37.4 (2) | C24—Fe2—C26—C25 | -37.1 (2) |
| C4—Fe1—C5—C1 | 119.1 (3) | C24—Fe2—C26—C27 | 82.0 (3) |
| C7—Fe1—C5—C1 | 170.6 (3) | C25—Fe2—C26—C27 | 119.1 (4) |
| C7—Fe1—C5—C4 | 51.5 (4) | C27—Fe2—C26—C25 | -119.1 (4) |
| C8—Fe1—C5—C1 | -155.6 (2) | C28—Fe2—C26—C25 | -81.1 (3) |

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| C8—Fe1—C5—C4 | 85.3 (2) | C28—Fe2—C26—C27 | 38.0 (3) |
| C9—Fe1—C5—C1 | -113.1 (2) | C19—Fe2—C27—C26 | -168.9 (3) |
| C9—Fe1—C5—C4 | 127.8 (2) | C19—Fe2—C27—C28 | -50.5 (5) |
| C10—Fe1—C5—C1 | -73.6 (3) | C21—Fe2—C27—C26 | 73.6 (3) |
| C10—Fe1—C5—C4 | 167.3 (2) | C21—Fe2—C27—C28 | -168.0 (3) |
| C1—Fe1—C6—C7 | 169.5 (2) | C22—Fe2—C27—C26 | 114.1 (3) |
| C1—Fe1—C6—C10 | -70.2 (3) | C22—Fe2—C27—C28 | -127.5 (3) |
| C2—Fe1—C6—C7 | 127.9 (2) | C23—Fe2—C27—C26 | 156.9 (3) |
| C2—Fe1—C6—C10 | -111.7 (2) | C23—Fe2—C27—C28 | -84.7 (3) |
| C3—Fe1—C6—C7 | 83.5 (3) | C24—Fe2—C27—C26 | -80.8 (3) |
| C3—Fe1—C6—C10 | -156.1 (2) | C24—Fe2—C27—C28 | 37.6 (3) |
| C4—Fe1—C6—C7 | 45.5 (4) | C25—Fe2—C27—C26 | -37.6 (3) |
| C4—Fe1—C6—C10 | 165.8 (3) | C25—Fe2—C27—C28 | 80.8 (3) |
| C7—Fe1—C6—C10 | 120.4 (3) | C26—Fe2—C27—C28 | 118.4 (4) |
| C8—Fe1—C6—C7 | -38.5 (2) | C28—Fe2—C27—C26 | -118.4 (4) |
| C8—Fe1—C6—C10 | 82.0 (2) | C19—Fe2—C28—C24 | -84.2 (3) |
| C9—Fe1—C6—C7 | -82.2 (2) | C19—Fe2—C28—C27 | 156.4 (3) |
| C9—Fe1—C6—C10 | 38.2 (2) | C20—Fe2—C28—C24 | -49.4 (6) |
| C10—Fe1—C6—C7 | -120.4 (3) | C20—Fe2—C28—C27 | -168.8 (4) |
| C2—Fe1—C7—C6 | -74.5 (3) | C22—Fe2—C28—C24 | -168.4 (2) |
| C2—Fe1—C7—C8 | 167.7 (2) | C22—Fe2—C28—C27 | 72.2 (4) |
| C3—Fe1—C7—C6 | -114.2 (2) | C23—Fe2—C28—C24 | -127.0 (3) |
| C3—Fe1—C7—C8 | 128.0 (2) | C23—Fe2—C28—C27 | 113.6 (3) |
| C4—Fe1—C7—C6 | -157.1 (2) | C24—Fe2—C28—C27 | -119.4 (5) |
| C4—Fe1—C7—C8 | 85.1 (3) | C25—Fe2—C28—C24 | 37.7 (3) |
| C5—Fe1—C7—C6 | 168.2 (3) | C25—Fe2—C28—C27 | -81.7 (3) |
| C5—Fe1—C7—C8 | 50.3 (4) | C26—Fe2—C28—C24 | 81.5 (3) |
| C6—Fe1—C7—C8 | -117.9 (3) | C26—Fe2—C28—C27 | -38.0 (3) |
| C8—Fe1—C7—C6 | 117.9 (3) | C27—Fe2—C28—C24 | 119.4 (5) |
| C9—Fe1—C7—C6 | 80.8 (2) | C11—N1—C12—C13 | -81.2 (4) |
| C9—Fe1—C7—C8 | -37.1 (2) | C11—N1—C12—C17 | 156.6 (3) |
| C10—Fe1—C7—C6 | 36.9 (2) | C12—N1—C11—C1 | 178.4 (3) |
| C10—Fe1—C7—C8 | -81.0 (2) | C18—N2—C17—C12 | 160.1 (3) |
| C1—Fe1—C8—C7 | 173.5 (3) | C18—N2—C17—C16 | -74.6 (4) |
| C1—Fe1—C8—C9 | 53.4 (4) | C17—N2—C18—C19 | 168.3 (3) |
| C3—Fe1—C8—C7 | -71.8 (3) | C11—C1—C2—Fe1 | -122.8 (3) |
| C3—Fe1—C8—C9 | 168.1 (2) | C11—C1—C2—C3 | 177.7 (3) |
| C4—Fe1—C8—C7 | -111.0 (2) | C5—C1—C2—C3 | -0.5 (4) |
| C4—Fe1—C8—C9 | 128.9 (2) | C11—C1—C5—C4 | -178.3 (3) |
| C5—Fe1—C8—C7 | -153.9 (2) | Fe1—C1—C11—N1 | 49.8 (4) |
| C5—Fe1—C8—C9 | 86.0 (3) | C2—C1—C11—N1 | 141.3 (3) |
| C6—Fe1—C8—C7 | 38.4 (2) | C5—C1—C11—N1 | -40.8 (5) |
| C6—Fe1—C8—C9 | -81.8 (3) | Fe1—C1—C5—C4 | 59.1 (2) |
| C7—Fe1—C8—C9 | -120.1 (3) | Fe1—C1—C2—C3 | -59.4 (3) |
| C9—Fe1—C8—C7 | 120.1 (3) | C5—C1—C2—Fe1 | 58.9 (2) |
| C10—Fe1—C8—C7 | 82.0 (2) | C2—C1—C5—C4 | 0.0 (4) |
| C10—Fe1—C8—C9 | -38.1 (2) | C11—C1—C5—Fe1 | 122.6 (3) |
| C1—Fe1—C9—C8 | -153.0 (2) | C2—C1—C5—Fe1 | -59.1 (2) |

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| C1—Fe1—C9—C10 | 88.3 (2) | C1—C2—C3—Fe1 | 59.5 (2) |
| C2—Fe1—C9—C8 | 174.2 (3) | C1—C2—C3—C4 | 0.9 (4) |
| C2—Fe1—C9—C10 | 55.5 (4) | Fe1—C2—C3—C4 | -58.6 (3) |
| C4—Fe1—C9—C8 | -69.8 (3) | C2—C3—C4—C5 | -0.9 (4) |
| C4—Fe1—C9—C10 | 171.5 (2) | C2—C3—C4—Fe1 | 59.0 (3) |
| C5—Fe1—C9—C8 | -110.3 (2) | Fe1—C3—C4—C5 | -59.9 (3) |
| C5—Fe1—C9—C10 | 131.0 (2) | Fe1—C4—C5—C1 | -59.7 (2) |
| C6—Fe1—C9—C8 | 81.0 (2) | C3—C4—C5—C1 | 0.6 (4) |
| C6—Fe1—C9—C10 | -37.8 (2) | C3—C4—C5—Fe1 | 60.3 (3) |
| C7—Fe1—C9—C8 | 37.2 (2) | Fe1—C6—C10—C9 | -59.4 (3) |
| C7—Fe1—C9—C10 | -81.5 (2) | C7—C6—C10—Fe1 | 58.3 (2) |
| C8—Fe1—C9—C10 | -118.7 (3) | C7—C6—C10—C9 | -1.1 (4) |
| C10—Fe1—C9—C8 | 118.7 (3) | C10—C6—C7—C8 | 1.4 (4) |
| C1—Fe1—C10—C6 | 131.2 (2) | Fe1—C6—C7—C8 | 60.1 (3) |
| C1—Fe1—C10—C9 | -110.2 (2) | C10—C6—C7—Fe1 | -58.7 (2) |
| C2—Fe1—C10—C6 | 87.8 (2) | Fe1—C7—C8—C9 | 59.5 (3) |
| C2—Fe1—C10—C9 | -153.6 (2) | C6—C7—C8—C9 | -1.2 (4) |
| C3—Fe1—C10—C6 | 50.2 (4) | C6—C7—C8—Fe1 | -60.7 (2) |
| C3—Fe1—C10—C9 | 168.8 (3) | C7—C8—C9—Fe1 | -59.3 (3) |
| C5—Fe1—C10—C6 | 172.8 (2) | C7—C8—C9—C10 | 0.5 (4) |
| C5—Fe1—C10—C9 | -68.6 (3) | Fe1—C8—C9—C10 | 59.8 (3) |
| C6—Fe1—C10—C9 | 118.6 (3) | C8—C9—C10—Fe1 | -59.4 (3) |
| C7—Fe1—C10—C6 | -37.0 (2) | Fe1—C9—C10—C6 | 59.8 (2) |
| C7—Fe1—C10—C9 | 81.6 (2) | C8—C9—C10—C6 | 0.4 (4) |
| C8—Fe1—C10—C6 | -80.9 (2) | N1—C12—C13—C14 | -174.5 (3) |
| C8—Fe1—C10—C9 | 37.8 (2) | C17—C12—C13—C14 | -53.7 (5) |
| C9—Fe1—C10—C6 | -118.6 (3) | N1—C12—C17—N2 | -59.7 (4) |
| C20—Fe2—C19—C18 | -121.8 (4) | N1—C12—C17—C16 | 173.0 (3) |
| C20—Fe2—C19—C23 | 118.2 (3) | C13—C12—C17—N2 | 179.5 (3) |
| C21—Fe2—C19—C18 | -159.0 (4) | C13—C12—C17—C16 | 52.3 (5) |
| C21—Fe2—C19—C20 | -37.2 (2) | C12—C13—C14—C15 | 56.5 (5) |
| C21—Fe2—C19—C23 | 81.0 (2) | C13—C14—C15—C16 | -57.8 (6) |
| C22—Fe2—C19—C18 | 157.6 (3) | C14—C15—C16—C17 | 57.7 (5) |
| C22—Fe2—C19—C20 | -80.6 (2) | C15—C16—C17—N2 | -179.5 (3) |
| C22—Fe2—C19—C23 | 37.6 (2) | C15—C16—C17—C12 | -55.1 (5) |
| C23—Fe2—C19—C18 | 120.0 (4) | N2—C18—C19—Fe2 | 179.3 (2) |
| C23—Fe2—C19—C20 | -118.2 (3) | N2—C18—C19—C20 | 87.8 (4) |
| C24—Fe2—C19—C18 | -7.2 (3) | N2—C18—C19—C23 | -90.3 (4) |
| C24—Fe2—C19—C20 | 114.6 (2) | Fe2—C19—C20—C21 | 59.1 (3) |
| C24—Fe2—C19—C23 | -127.2 (2) | C18—C19—C20—Fe2 | 122.0 (4) |
| C25—Fe2—C19—C18 | -47.5 (4) | C18—C19—C20—C21 | -179.0 (3) |
| C25—Fe2—C19—C20 | 74.3 (3) | C23—C19—C20—Fe2 | -59.6 (2) |
| C25—Fe2—C19—C23 | -167.5 (2) | C23—C19—C20—C21 | -0.6 (4) |
| C27—Fe2—C19—C18 | 70.8 (5) | Fe2—C19—C23—C22 | -59.2 (3) |
| C27—Fe2—C19—C20 | -167.4 (3) | C18—C19—C23—Fe2 | -122.0 (4) |
| C27—Fe2—C19—C23 | -49.2 (4) | C18—C19—C23—C22 | 178.8 (3) |
| C28—Fe2—C19—C18 | 35.8 (4) | C20—C19—C23—Fe2 | 59.6 (2) |
| C28—Fe2—C19—C20 | 157.6 (2) | C20—C19—C23—C22 | 0.4 (4) |

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| C28—Fe2—C19—C23 | -84.2 (3) | Fe2—C20—C21—C22 | 59.7 (3) |
| C19—Fe2—C20—C21 | -119.8 (3) | C19—C20—C21—Fe2 | -59.2 (2) |
| C21—Fe2—C20—C19 | 119.8 (3) | C19—C20—C21—C22 | 0.5 (4) |
| C22—Fe2—C20—C19 | 82.1 (2) | Fe2—C21—C22—C23 | 59.7 (3) |
| C22—Fe2—C20—C21 | -37.7 (2) | C20—C21—C22—Fe2 | -59.9 (3) |
| C23—Fe2—C20—C19 | 38.0 (2) | C20—C21—C22—C23 | -0.3 (4) |
| C23—Fe2—C20—C21 | -81.7 (3) | Fe2—C22—C23—C19 | 59.7 (3) |
| C24—Fe2—C20—C19 | -84.1 (2) | C21—C22—C23—Fe2 | -59.8 (3) |
| C24—Fe2—C20—C21 | 156.2 (2) | C21—C22—C23—C19 | -0.1 (4) |
| C25—Fe2—C20—C19 | -126.5 (2) | Fe2—C24—C25—C26 | -59.3 (3) |
| C25—Fe2—C20—C21 | 113.7 (2) | C28—C24—C25—Fe2 | 60.4 (3) |
| C26—Fe2—C20—C19 | -167.6 (2) | C28—C24—C25—C26 | 1.1 (5) |
| C26—Fe2—C20—C21 | 72.6 (3) | Fe2—C24—C28—C27 | 59.6 (3) |
| C28—Fe2—C20—C19 | -49.4 (5) | C25—C24—C28—Fe2 | -60.8 (3) |
| C28—Fe2—C20—C21 | -169.1 (4) | C25—C24—C28—C27 | -1.2 (5) |
| C19—Fe2—C21—C20 | 37.5 (2) | Fe2—C25—C26—C27 | -59.5 (3) |
| C19—Fe2—C21—C22 | -81.3 (2) | C24—C25—C26—Fe2 | 59.0 (3) |
| C20—Fe2—C21—C22 | -118.8 (3) | C24—C25—C26—C27 | -0.5 (5) |
| C22—Fe2—C21—C20 | 118.8 (3) | Fe2—C26—C27—C28 | -59.9 (3) |
| C23—Fe2—C21—C20 | 81.1 (2) | C25—C26—C27—Fe2 | 59.7 (3) |
| C23—Fe2—C21—C22 | -37.7 (2) | C25—C26—C27—C28 | -0.2 (5) |
| C24—Fe2—C21—C20 | -51.3 (5) | Fe2—C27—C28—C24 | -59.2 (3) |
| C24—Fe2—C21—C22 | -170.1 (3) | C26—C27—C28—Fe2 | 60.1 (3) |
| C25—Fe2—C21—C20 | -84.8 (3) | C26—C27—C28—C24 | 0.9 (5) |
| C25—Fe2—C21—C22 | 156.4 (2) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------|-------|-------------|-------------|---------------|
| N1—H1A \cdots N2 | 0.90 | 2.36 | 2.848 (4) | 114 |