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# (*S*)-1-Ferrocenyl-3-hydroxy-3-phenylpropan-1-one

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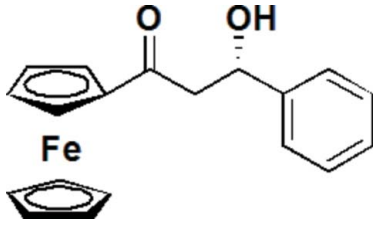
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.031; $wR$ factor = 0.066; data-to-parameter ratio = 13.6.

In the title compound, [Fe($C_5H_5$)($C_{14}H_{13}O_2$)], the dihedral angle between the phenyl ring and the unsubstituted cyclopetadienyl ring is 85.0 (2)°while that between the phenyl ring and the substituted cyclopetadienyl ring is 83.6 (2)°. The dihedral angle between the two cyclopenta-1,3-diene rings of the ferrocene unit is 2.2 (2)°. The molecules are stabilized by intermolecular O—H···O hydrogen-bonding interaction within the crystal lattice.

## Related literature

For the preparation, see: Patti & Pedotti (2006*a*); Hashiguchi *et al.* (1995). For use of the title compound in the preparation of chiral diols, see: Patti & Pedotti (2006*b*) and of phosphine ligands, see: Zhang *et al.* (2007).




## Experimental

### Crystal data

[Fe($C_5H_5$)($C_{14}H_{13}O_2$)]
$M_r$ = 334.18
Orthorhombic, $P2_12_12_1$
$a$ = 10.0609 (14) Å
$b$ = 10.6054 (15) Å
$c$ = 14.335 (2) Å
$V$ = 1529.5 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.99 mm$^{-1}$
$T$ = 296 K
0.34 × 0.28 × 0.18 mm

### Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.728, $T_{max}$ = 0.840
7586 measured reflections
2721 independent reflections
2424 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.066
$S$ = 1.06
2721 reflections
200 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$
Absolute structure: Flack (1983), 1146 Friedel pairs
Flack parameter: −0.004 (19)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O2$^{i}$ | 0.82 | 2.04 | 2.841 (3) | 166 |

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; 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: *Mercury* (Macrae *et al.*, 2006) and *ORTEP-3* (Farrugia, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PB2052).

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# supporting information

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## (*S*)-1-Ferrocenyl-3-hydroxy-3-phenylpropan-1-one

**Ping-An Wang**

### S1. Comment

The title compound, (*S*)-1-ferrocenyl-3-phenyl-3-hydroxypropane- 1-one, was obtained from the catalytic asymmetric transfer hydrogenation of 1-ferrocenyl-3-phenyl-1,3-dione with the mixed solution of $Et_3N$ and HCOOH by using Noyori's catalyst (Hashiguchi *et al.* 1995) and it was used for the preparation of chiral diols (Patti *et al.* 2006b) and phosphine ligands (Zhang *et al.* 2007).

In the title compound, $C_{19}H_{18}FeO_2$, the dihedral angle between the phenyl ring and the plane defined by the cyclopetadienyl ring ( C15, C16, C17,C18 and C19) is 85.0°. However, the dihedral angle between the phenyl ring and the plane defined by the second Cp ring (C10, C11, C12, C13 and C14) is 83.6°. The dihedral angle between the two cyclopenta-1,3-diene rings of the ferrocene moiety is 2.21°. The packing of molecules is stabilized by intermolecular O—H···O hydrogen bonds.

### S2. Experimental

A mixture of $[RuCl_2(</>p\text{-cymene})]_2$ (20.0 mg, 0.030 mmol) and (1</>S,2</>S)-[</>N-(tosyl)- 1,2-diphenylethylendiamine](22.5 mg, 0.061 mmol) in 2-propanol (1.0 $cm^3$) was heated at 80°C for 30 min under argon, then the solvent was removed under vacuum. the mixed solution of $Et_3N$ and HCOOH (1.5 $cm^3$) and 1-ferrocenyl-3-phenyl- 1,3-dione (0.34 g, 1.2 mmol) were added to the Ru-complex and the mixture stirred at 50°C while monitoring the reaction progress by thin layer chromatography. After 1.0 h, the solution was diluted with water (3.0 $cm^3$) and extracted with ethyl acetate (2×, 20.0 $cm^3$). The organic layer was washed with brine (2×, 10.0 $cm^3$), dried over $Na_2SO_4$ and taken to dryness under vacuum. The residue was purified on silica gel column to give the title compound (0.31 g, 92% yield), and also produced (1</>S,3</>S)-1-ferrocenyl-3-phenyl- 1,3-dihydroxypropane (11.6 mg, 3.5% yield). The melting point and the spectroscopic data of the title compound were consisted with the reported literature (Patti & Pedotti, 2006a).

### S3. Refinement

All H atoms were placed in calculated positions and refined as riding, with C—H = 0.93–0.98Å and with $U_{iso}$(H) = 1.2$U_{eq}$(C); with $U_{iso}$(H) = 1.5$U_{eq}$(O).

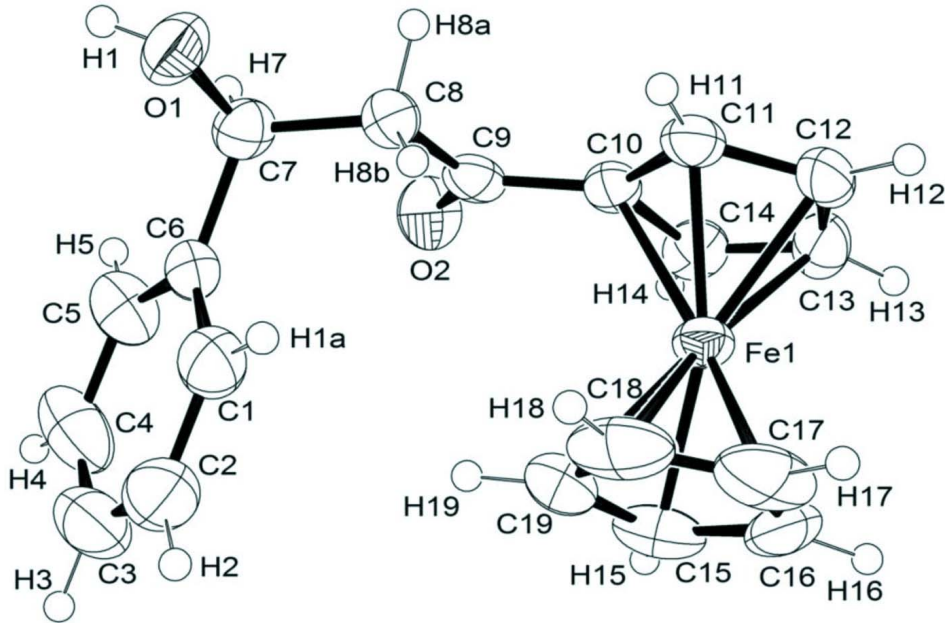


**Figure 1**

The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

### (*S*)-1-Ferrocenyl-3-hydroxy-3-phenylpropan-1-one

*Crystal data*

$[Fe(C_5H_5)(C_{14}H_{13}O_2)]$
$M_r = 334.18$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 10.0609\ (14)$ Å
$b = 10.6054\ (15)$ Å
$c = 14.335\ (2)$ Å
$V = 1529.5\ (4)$ Å$^3$
$Z = 4$
$F(000) = 696$
$D_x = 1.451$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2427 reflections
$\theta = 2.5$–$23.9°$
$\mu = 0.99$ mm$^{-1}$
$T = 296$ K
Block, orange-red
0.34 × 0.28 × 0.18 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.728$, $T_{max} = 0.840$
7586 measured reflections
2721 independent reflections
2424 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.4°$
$h = -8 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -17 \rightarrow 14$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.066$
$S = 1.06$
2721 reflections
200 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
$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å$^{-3}$
$\Delta\rho_{min} = -0.22$ e Å$^{-3}$
Absolute structure: Flack (1983), **1146 Friedel pairs**
Absolute structure parameter: −0.004 (19)

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Fe1 | 0.11375 (4) | 0.33401 (4) | 0.18512 (2) | 0.03633 (12) |
| O1 | 0.57703 (19) | 0.63931 (19) | 0.04641 (14) | 0.0539 (6) |
| H1 | 0.6135 | 0.7011 | 0.0234 | 0.081* |
| O2 | 0.1578 (2) | 0.62907 (17) | 0.03540 (14) | 0.0533 (6) |
| C1 | 0.4265 (3) | 0.6868 (3) | 0.2293 (2) | 0.0549 (8) |
| H1A | 0.4579 | 0.6046 | 0.2348 | 0.066* |
| C2 | 0.4006 (4) | 0.7564 (4) | 0.3096 (2) | 0.0698 (10) |
| H2 | 0.4136 | 0.7208 | 0.3682 | 0.084* |
| C3 | 0.3556 (4) | 0.8786 (4) | 0.3014 (3) | 0.0771 (12) |
| H3 | 0.3384 | 0.9258 | 0.3548 | 0.092* |
| C4 | 0.3361 (4) | 0.9309 (4) | 0.2153 (3) | 0.0760 (12) |
| H4 | 0.3062 | 1.0136 | 0.2100 | 0.091* |
| C5 | 0.3611 (3) | 0.8600 (3) | 0.1359 (2) | 0.0572 (9) |
| H5 | 0.3471 | 0.8956 | 0.0774 | 0.069* |
| C6 | 0.4066 (3) | 0.7371 (3) | 0.14234 (18) | 0.0394 (7) |
| C7 | 0.4371 (3) | 0.6624 (3) | 0.05389 (18) | 0.0420 (6) |
| H7 | 0.4081 | 0.7114 | −0.0004 | 0.050* |
| C8 | 0.3721 (3) | 0.5344 (2) | 0.05076 (18) | 0.0405 (6) |
| H8A | 0.4048 | 0.4901 | −0.0038 | 0.049* |
| H8B | 0.4005 | 0.4871 | 0.1052 | 0.049* |
| C9 | 0.2226 (3) | 0.5330 (3) | 0.04789 (17) | 0.0382 (7) |
| C10 | 0.1570 (3) | 0.4105 (3) | 0.05858 (18) | 0.0364 (7) |
| C11 | 0.2179 (3) | 0.2888 (3) | 0.06855 (18) | 0.0397 (7) |
| H11 | 0.3134 | 0.2712 | 0.0657 | 0.048* |
| C12 | 0.1172 (4) | 0.1992 (3) | 0.08209 (17) | 0.0472 (8) |
| H12 | 0.1309 | 0.1086 | 0.0918 | 0.057* |
| C13 | −0.0068 (4) | 0.2617 (3) | 0.08331 (19) | 0.0510 (9) |
| H13 | −0.0936 | 0.2220 | 0.0930 | 0.061* |
| C14 | 0.0165 (3) | 0.3913 (3) | 0.06844 (19) | 0.0460 (8) |

| | | | | |
|---|---|---|---|---|
| H14 | −0.0517 | 0.4572 | 0.0656 | 0.055* |
| C15 | 0.0302 (4) | 0.4278 (4) | 0.2937 (2) | 0.0614 (11) |
| H15 | −0.0459 | 0.4851 | 0.2894 | 0.074* |
| C16 | 0.0229 (4) | 0.2989 (4) | 0.3087 (2) | 0.0697 (12) |
| H16 | −0.0583 | 0.2494 | 0.3181 | 0.084* |
| C17 | 0.1545 (5) | 0.2528 (4) | 0.3103 (2) | 0.0751 (13) |
| H17 | 0.1818 | 0.1652 | 0.3208 | 0.090* |
| C18 | 0.2385 (3) | 0.3553 (4) | 0.2957 (2) | 0.0682 (11) |
| H18 | 0.3358 | 0.3520 | 0.2932 | 0.082* |
| C19 | 0.1618 (4) | 0.4624 (4) | 0.2855 (2) | 0.0570 (9) |
| H19 | 0.1950 | 0.5480 | 0.2746 | 0.068* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Fe1 | 0.0403 (2) | 0.0419 (2) | 0.02675 (18) | −0.0006 (2) | 0.00075 (19) | −0.00136 (19) |
| O1 | 0.0498 (13) | 0.0496 (14) | 0.0624 (13) | −0.0068 (10) | 0.0158 (10) | 0.0073 (11) |
| O2 | 0.0576 (14) | 0.0395 (12) | 0.0629 (14) | 0.0074 (11) | −0.0070 (11) | 0.0096 (10) |
| C1 | 0.061 (2) | 0.056 (2) | 0.0474 (17) | −0.0109 (18) | −0.0026 (15) | 0.0007 (17) |
| C2 | 0.067 (2) | 0.098 (3) | 0.0443 (19) | −0.024 (2) | −0.005 (2) | −0.002 (2) |
| C3 | 0.053 (2) | 0.104 (3) | 0.074 (3) | −0.011 (2) | 0.004 (2) | −0.044 (2) |
| C4 | 0.063 (2) | 0.065 (2) | 0.100 (3) | 0.009 (2) | −0.016 (2) | −0.036 (2) |
| C5 | 0.058 (2) | 0.052 (2) | 0.061 (2) | 0.0040 (18) | −0.0118 (17) | −0.0081 (16) |
| C6 | 0.0406 (18) | 0.0392 (15) | 0.0385 (15) | −0.0068 (14) | −0.0006 (13) | −0.0025 (12) |
| C7 | 0.0494 (17) | 0.0373 (15) | 0.0392 (14) | 0.0004 (15) | 0.0046 (13) | 0.0062 (15) |
| C8 | 0.0461 (17) | 0.0339 (14) | 0.0414 (15) | −0.0008 (15) | 0.0053 (15) | −0.0015 (12) |
| C9 | 0.0529 (18) | 0.0401 (17) | 0.0215 (13) | 0.0033 (15) | −0.0007 (13) | −0.0018 (12) |
| C10 | 0.0486 (19) | 0.0374 (15) | 0.0233 (14) | −0.0020 (14) | −0.0010 (13) | 0.0013 (12) |
| C11 | 0.0526 (19) | 0.0377 (17) | 0.0289 (15) | 0.0038 (15) | 0.0048 (14) | −0.0011 (12) |
| C12 | 0.074 (2) | 0.0366 (15) | 0.0312 (14) | −0.0089 (19) | 0.0015 (16) | −0.0028 (11) |
| C13 | 0.061 (2) | 0.057 (2) | 0.0347 (18) | −0.0235 (18) | −0.0100 (16) | 0.0012 (15) |
| C14 | 0.0437 (18) | 0.061 (2) | 0.0331 (17) | −0.0048 (16) | −0.0093 (15) | 0.0033 (15) |
| C15 | 0.062 (2) | 0.082 (3) | 0.040 (2) | 0.022 (2) | 0.0048 (17) | −0.0185 (18) |
| C16 | 0.079 (3) | 0.098 (3) | 0.0317 (17) | −0.039 (2) | 0.018 (2) | −0.007 (2) |
| C17 | 0.140 (4) | 0.059 (2) | 0.0259 (17) | 0.028 (3) | −0.006 (2) | 0.0069 (18) |
| C18 | 0.054 (2) | 0.121 (4) | 0.0298 (18) | 0.008 (2) | −0.0092 (14) | −0.011 (2) |
| C19 | 0.072 (2) | 0.062 (2) | 0.0368 (18) | −0.010 (2) | −0.0026 (15) | −0.0132 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Fe1—C16 | 2.028 (3) | C7—C8 | 1.508 (4) |
| Fe1—C15 | 2.029 (3) | C7—H7 | 0.9800 |
| Fe1—C11 | 2.030 (3) | C8—C9 | 1.504 (4) |
| Fe1—C14 | 2.031 (3) | C8—H8A | 0.9700 |
| Fe1—C17 | 2.032 (3) | C8—H8B | 0.9700 |
| Fe1—C10 | 2.034 (3) | C9—C10 | 1.466 (4) |
| Fe1—C18 | 2.034 (3) | C10—C14 | 1.435 (4) |
| Fe1—C19 | 2.038 (3) | C10—C11 | 1.436 (4) |

| | | | |
|---|---|---|---|
| Fe1—C13 | 2.047 (3) | C11—C12 | 1.402 (4) |
| Fe1—C12 | 2.056 (3) | C11—H11 | 0.9800 |
| O1—C7 | 1.433 (3) | C12—C13 | 1.413 (5) |
| O1—H1 | 0.8200 | C12—H12 | 0.9800 |
| O2—C9 | 1.223 (3) | C13—C14 | 1.410 (4) |
| C1—C6 | 1.371 (4) | C13—H13 | 0.9800 |
| C1—C2 | 1.392 (4) | C14—H14 | 0.9800 |
| C1—H1A | 0.9300 | C15—C19 | 1.379 (5) |
| C2—C3 | 1.377 (5) | C15—C16 | 1.386 (5) |
| C2—H2 | 0.9300 | C15—H15 | 0.9800 |
| C3—C4 | 1.368 (5) | C16—C17 | 1.412 (5) |
| C3—H3 | 0.9300 | C16—H16 | 0.9800 |
| C4—C5 | 1.388 (4) | C17—C18 | 1.393 (5) |
| C4—H4 | 0.9300 | C17—H17 | 0.9800 |
| C5—C6 | 1.385 (4) | C18—C19 | 1.381 (5) |
| C5—H5 | 0.9300 | C18—H18 | 0.9800 |
| C6—C7 | 1.526 (4) | C19—H19 | 0.9800 |

| | | | |
|---|---|---|---|
| C16—Fe1—C15 | 39.94 (15) | C9—C8—C7 | 116.3 (2) |
| C16—Fe1—C11 | 155.28 (15) | C9—C8—H8A | 108.2 |
| C15—Fe1—C11 | 163.96 (14) | C7—C8—H8A | 108.2 |
| C16—Fe1—C14 | 123.86 (16) | C9—C8—H8B | 108.2 |
| C15—Fe1—C14 | 106.59 (13) | C7—C8—H8B | 108.2 |
| C11—Fe1—C14 | 68.99 (13) | H8A—C8—H8B | 107.4 |
| C16—Fe1—C17 | 40.70 (16) | O2—C9—C10 | 120.9 (3) |
| C15—Fe1—C17 | 67.29 (15) | O2—C9—C8 | 122.0 (3) |
| C11—Fe1—C17 | 121.51 (14) | C10—C9—C8 | 117.1 (2) |
| C14—Fe1—C17 | 162.04 (16) | C14—C10—C11 | 106.5 (3) |
| C16—Fe1—C10 | 161.55 (15) | C14—C10—C9 | 125.5 (3) |
| C15—Fe1—C10 | 125.25 (14) | C11—C10—C9 | 127.9 (3) |
| C11—Fe1—C10 | 41.39 (10) | C14—C10—Fe1 | 69.21 (17) |
| C14—Fe1—C10 | 41.34 (12) | C11—C10—Fe1 | 69.15 (16) |
| C17—Fe1—C10 | 155.97 (17) | C9—C10—Fe1 | 122.89 (19) |
| C16—Fe1—C18 | 67.55 (15) | C12—C11—C10 | 108.3 (3) |
| C15—Fe1—C18 | 66.67 (15) | C12—C11—Fe1 | 70.94 (16) |
| C11—Fe1—C18 | 110.42 (14) | C10—C11—Fe1 | 69.46 (16) |
| C14—Fe1—C18 | 154.93 (16) | C12—C11—H11 | 125.8 |
| C17—Fe1—C18 | 40.05 (15) | C10—C11—H11 | 125.8 |
| C10—Fe1—C18 | 121.24 (14) | Fe1—C11—H11 | 125.8 |
| C16—Fe1—C19 | 67.24 (14) | C11—C12—C13 | 108.8 (3) |
| C15—Fe1—C19 | 39.62 (13) | C11—C12—Fe1 | 68.93 (15) |
| C11—Fe1—C19 | 128.06 (13) | C13—C12—Fe1 | 69.50 (17) |
| C14—Fe1—C19 | 119.70 (14) | C11—C12—H12 | 125.6 |
| C17—Fe1—C19 | 67.18 (15) | C13—C12—H12 | 125.6 |
| C10—Fe1—C19 | 108.20 (13) | Fe1—C12—H12 | 125.6 |
| C18—Fe1—C19 | 39.65 (14) | C14—C13—C12 | 108.0 (3) |
| C16—Fe1—C13 | 106.68 (14) | C14—C13—Fe1 | 69.16 (19) |
| C15—Fe1—C13 | 119.02 (15) | C12—C13—Fe1 | 70.21 (18) |

| | | | |
|---|---|---|---|
| C11—Fe1—C13 | 68.29 (12) | C14—C13—H13 | 126.0 |
| C14—Fe1—C13 | 40.47 (11) | C12—C13—H13 | 126.0 |
| C17—Fe1—C13 | 126.19 (16) | Fe1—C13—H13 | 126.0 |
| C10—Fe1—C13 | 68.90 (12) | C13—C14—C10 | 108.4 (3) |
| C18—Fe1—C13 | 164.30 (16) | C13—C14—Fe1 | 70.37 (19) |
| C19—Fe1—C13 | 153.36 (15) | C10—C14—Fe1 | 69.45 (17) |
| C16—Fe1—C12 | 120.49 (13) | C13—C14—H14 | 125.8 |
| C15—Fe1—C12 | 154.01 (15) | C10—C14—H14 | 125.8 |
| C11—Fe1—C12 | 40.13 (11) | Fe1—C14—H14 | 125.8 |
| C14—Fe1—C12 | 67.96 (13) | C19—C15—C16 | 109.1 (4) |
| C17—Fe1—C12 | 109.65 (14) | C19—C15—Fe1 | 70.6 (2) |
| C10—Fe1—C12 | 68.47 (11) | C16—C15—Fe1 | 70.0 (2) |
| C18—Fe1—C12 | 128.76 (15) | C19—C15—H15 | 125.5 |
| C19—Fe1—C12 | 165.30 (15) | C16—C15—H15 | 125.5 |
| C13—Fe1—C12 | 40.29 (14) | Fe1—C15—H15 | 125.5 |
| C7—O1—H1 | 109.5 | C15—C16—C17 | 107.1 (3) |
| C6—C1—C2 | 121.2 (3) | C15—C16—Fe1 | 70.1 (2) |
| C6—C1—H1A | 119.4 | C17—C16—Fe1 | 69.8 (2) |
| C2—C1—H1A | 119.4 | C15—C16—H16 | 126.4 |
| C3—C2—C1 | 119.4 (3) | C17—C16—H16 | 126.4 |
| C3—C2—H2 | 120.3 | Fe1—C16—H16 | 126.4 |
| C1—C2—H2 | 120.3 | C18—C17—C16 | 107.3 (3) |
| C4—C3—C2 | 120.4 (3) | C18—C17—Fe1 | 70.0 (2) |
| C4—C3—H3 | 119.8 | C16—C17—Fe1 | 69.5 (2) |
| C2—C3—H3 | 119.8 | C18—C17—H17 | 126.4 |
| C3—C4—C5 | 119.7 (3) | C16—C17—H17 | 126.4 |
| C3—C4—H4 | 120.2 | Fe1—C17—H17 | 126.4 |
| C5—C4—H4 | 120.2 | C19—C18—C17 | 108.6 (3) |
| C6—C5—C4 | 121.0 (3) | C19—C18—Fe1 | 70.34 (18) |
| C6—C5—H5 | 119.5 | C17—C18—Fe1 | 69.9 (2) |
| C4—C5—H5 | 119.5 | C19—C18—H18 | 125.7 |
| C1—C6—C5 | 118.4 (3) | C17—C18—H18 | 125.7 |
| C1—C6—C7 | 121.6 (3) | Fe1—C18—H18 | 125.7 |
| C5—C6—C7 | 120.0 (2) | C15—C19—C18 | 108.0 (4) |
| O1—C7—C8 | 105.7 (2) | C15—C19—Fe1 | 69.8 (2) |
| O1—C7—C6 | 110.4 (2) | C18—C19—Fe1 | 70.01 (19) |
| C8—C7—C6 | 113.9 (2) | C15—C19—H19 | 126.0 |
| O1—C7—H7 | 108.9 | C18—C19—H19 | 126.0 |
| C8—C7—H7 | 108.9 | Fe1—C19—H19 | 126.0 |
| C6—C7—H7 | 108.9 | | |

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| C6—C1—C2—C3 | −0.8 (5) | C9—C10—C14—Fe1 | −116.3 (3) |
| C1—C2—C3—C4 | 0.2 (6) | C16—Fe1—C14—C13 | −75.3 (3) |
| C2—C3—C4—C5 | 0.4 (6) | C15—Fe1—C14—C13 | −115.5 (2) |
| C3—C4—C5—C6 | −0.5 (5) | C11—Fe1—C14—C13 | 80.8 (2) |
| C2—C1—C6—C5 | 0.7 (5) | C17—Fe1—C14—C13 | −48.3 (6) |
| C2—C1—C6—C7 | 178.8 (3) | C10—Fe1—C14—C13 | 119.5 (3) |
| C4—C5—C6—C1 | −0.1 (5) | C18—Fe1—C14—C13 | 174.3 (3) |

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| C4—C5—C6—C7 | −178.2 (3) | C19—Fe1—C14—C13 | −156.5 (2) |
| C1—C6—C7—O1 | −65.9 (4) | C12—Fe1—C14—C13 | 37.5 (2) |
| C5—C6—C7—O1 | 112.2 (3) | C16—Fe1—C14—C10 | 165.20 (19) |
| C1—C6—C7—C8 | 52.7 (4) | C15—Fe1—C14—C10 | 125.0 (2) |
| C5—C6—C7—C8 | −129.2 (3) | C11—Fe1—C14—C10 | −38.73 (18) |
| O1—C7—C8—C9 | −174.2 (2) | C17—Fe1—C14—C10 | −167.8 (4) |
| C6—C7—C8—C9 | 64.5 (3) | C18—Fe1—C14—C10 | 54.8 (4) |
| C7—C8—C9—O2 | 10.1 (4) | C19—Fe1—C14—C10 | 84.0 (2) |
| C7—C8—C9—C10 | −171.3 (2) | C13—Fe1—C14—C10 | −119.5 (3) |
| O2—C9—C10—C14 | −8.9 (4) | C12—Fe1—C14—C10 | −82.0 (2) |
| C8—C9—C10—C14 | 172.5 (3) | C16—Fe1—C15—C19 | 119.8 (4) |
| O2—C9—C10—C11 | 176.3 (3) | C11—Fe1—C15—C19 | −45.4 (6) |
| C8—C9—C10—C11 | −2.3 (4) | C14—Fe1—C15—C19 | −116.8 (2) |
| O2—C9—C10—Fe1 | −95.6 (3) | C17—Fe1—C15—C19 | 81.1 (3) |
| C8—C9—C10—Fe1 | 85.8 (3) | C10—Fe1—C15—C19 | −75.3 (3) |
| C16—Fe1—C10—C14 | −42.1 (5) | C18—Fe1—C15—C19 | 37.5 (2) |
| C15—Fe1—C10—C14 | −74.1 (2) | C13—Fe1—C15—C19 | −158.9 (2) |
| C11—Fe1—C10—C14 | 118.0 (3) | C12—Fe1—C15—C19 | 169.6 (3) |
| C17—Fe1—C10—C14 | 170.8 (3) | C11—Fe1—C15—C16 | −165.2 (4) |
| C18—Fe1—C10—C14 | −156.1 (2) | C14—Fe1—C15—C16 | 123.4 (3) |
| C19—Fe1—C10—C14 | −114.6 (2) | C17—Fe1—C15—C16 | −38.7 (2) |
| C13—Fe1—C10—C14 | 37.26 (19) | C10—Fe1—C15—C16 | 164.9 (2) |
| C12—Fe1—C10—C14 | 80.7 (2) | C18—Fe1—C15—C16 | −82.4 (3) |
| C16—Fe1—C10—C11 | −160.1 (4) | C19—Fe1—C15—C16 | −119.8 (4) |
| C15—Fe1—C10—C11 | 168.0 (2) | C13—Fe1—C15—C16 | 81.3 (3) |
| C14—Fe1—C10—C11 | −118.0 (3) | C12—Fe1—C15—C16 | 49.8 (4) |
| C17—Fe1—C10—C11 | 52.9 (4) | C19—C15—C16—C17 | 0.4 (5) |
| C18—Fe1—C10—C11 | 85.9 (2) | Fe1—C15—C16—C17 | 60.3 (3) |
| C19—Fe1—C10—C11 | 127.47 (19) | C19—C15—C16—Fe1 | −59.9 (3) |
| C13—Fe1—C10—C11 | −80.69 (19) | C11—Fe1—C16—C15 | 170.3 (3) |
| C12—Fe1—C10—C11 | −37.30 (18) | C14—Fe1—C16—C15 | −74.6 (3) |
| C16—Fe1—C10—C9 | 77.5 (5) | C17—Fe1—C16—C15 | 117.8 (3) |
| C15—Fe1—C10—C9 | 45.5 (3) | C10—Fe1—C16—C15 | −42.4 (5) |
| C11—Fe1—C10—C9 | −122.5 (3) | C18—Fe1—C16—C15 | 80.0 (3) |
| C14—Fe1—C10—C9 | 119.6 (3) | C19—Fe1—C16—C15 | 36.9 (2) |
| C17—Fe1—C10—C9 | −69.6 (4) | C13—Fe1—C16—C15 | −115.5 (2) |
| C18—Fe1—C10—C9 | −36.6 (3) | C12—Fe1—C16—C15 | −157.1 (2) |
| C19—Fe1—C10—C9 | 5.0 (3) | C15—Fe1—C16—C17 | −117.8 (3) |
| C13—Fe1—C10—C9 | 156.8 (3) | C11—Fe1—C16—C17 | 52.5 (4) |
| C12—Fe1—C10—C9 | −159.8 (3) | C14—Fe1—C16—C17 | 167.6 (2) |
| C14—C10—C11—C12 | 1.1 (3) | C10—Fe1—C16—C17 | −160.2 (4) |
| C9—C10—C11—C12 | 176.7 (3) | C18—Fe1—C16—C17 | −37.8 (2) |
| Fe1—C10—C11—C12 | 60.56 (18) | C19—Fe1—C16—C17 | −80.9 (2) |
| C14—C10—C11—Fe1 | −59.4 (2) | C13—Fe1—C16—C17 | 126.7 (2) |
| C9—C10—C11—Fe1 | 116.1 (3) | C12—Fe1—C16—C17 | 85.0 (3) |
| C16—Fe1—C11—C12 | 46.0 (4) | C15—C16—C17—C18 | −0.3 (5) |
| C15—Fe1—C11—C12 | −157.1 (5) | Fe1—C16—C17—C18 | 60.1 (3) |
| C14—Fe1—C11—C12 | −80.3 (2) | C15—C16—C17—Fe1 | −60.5 (3) |

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| C17—Fe1—C11—C12 | 83.4 (3) | C16—Fe1—C17—C18 | −118.2 (3) |
| C10—Fe1—C11—C12 | −119.0 (2) | C15—Fe1—C17—C18 | −80.2 (2) |
| C18—Fe1—C11—C12 | 126.5 (2) | C11—Fe1—C17—C18 | 84.7 (2) |
| C19—Fe1—C11—C12 | 167.8 (2) | C14—Fe1—C17—C18 | −153.5 (4) |
| C13—Fe1—C11—C12 | −36.72 (19) | C10—Fe1—C17—C18 | 46.5 (4) |
| C16—Fe1—C11—C10 | 165.0 (3) | C19—Fe1—C17—C18 | −37.1 (2) |
| C15—Fe1—C11—C10 | −38.1 (6) | C13—Fe1—C17—C18 | 169.5 (2) |
| C14—Fe1—C11—C10 | 38.68 (18) | C12—Fe1—C17—C18 | 127.5 (2) |
| C17—Fe1—C11—C10 | −157.6 (2) | C15—Fe1—C17—C16 | 38.0 (2) |
| C18—Fe1—C11—C10 | −114.5 (2) | C11—Fe1—C17—C16 | −157.1 (2) |
| C19—Fe1—C11—C10 | −73.2 (2) | C14—Fe1—C17—C16 | −35.3 (6) |
| C13—Fe1—C11—C10 | 82.28 (19) | C10—Fe1—C17—C16 | 164.7 (3) |
| C12—Fe1—C11—C10 | 119.0 (2) | C18—Fe1—C17—C16 | 118.2 (3) |
| C10—C11—C12—C13 | −1.5 (3) | C19—Fe1—C17—C16 | 81.1 (2) |
| Fe1—C11—C12—C13 | 58.18 (19) | C13—Fe1—C17—C16 | −72.2 (3) |
| C10—C11—C12—Fe1 | −59.63 (19) | C12—Fe1—C17—C16 | −114.3 (2) |
| C16—Fe1—C12—C11 | −159.55 (19) | C16—C17—C18—C19 | 0.2 (4) |
| C15—Fe1—C12—C11 | 165.8 (3) | Fe1—C17—C18—C19 | 59.9 (2) |
| C14—Fe1—C12—C11 | 83.1 (2) | C16—C17—C18—Fe1 | −59.8 (3) |
| C17—Fe1—C12—C11 | −115.9 (2) | C16—Fe1—C18—C19 | −80.9 (2) |
| C10—Fe1—C12—C11 | 38.44 (16) | C15—Fe1—C18—C19 | −37.4 (2) |
| C18—Fe1—C12—C11 | −75.0 (2) | C11—Fe1—C18—C19 | 125.6 (2) |
| C19—Fe1—C12—C11 | −41.2 (5) | C14—Fe1—C18—C19 | 41.7 (4) |
| C13—Fe1—C12—C11 | 120.8 (2) | C17—Fe1—C18—C19 | −119.4 (3) |
| C16—Fe1—C12—C13 | 79.7 (2) | C10—Fe1—C18—C19 | 80.8 (2) |
| C15—Fe1—C12—C13 | 45.0 (4) | C13—Fe1—C18—C19 | −152.1 (5) |
| C11—Fe1—C12—C13 | −120.8 (2) | C12—Fe1—C18—C19 | 167.19 (19) |
| C14—Fe1—C12—C13 | −37.68 (18) | C16—Fe1—C18—C17 | 38.4 (2) |
| C17—Fe1—C12—C13 | 123.3 (2) | C15—Fe1—C18—C17 | 81.9 (2) |
| C10—Fe1—C12—C13 | −82.36 (19) | C11—Fe1—C18—C17 | −115.1 (2) |
| C18—Fe1—C12—C13 | 164.2 (2) | C14—Fe1—C18—C17 | 161.1 (3) |
| C19—Fe1—C12—C13 | −161.9 (5) | C10—Fe1—C18—C17 | −159.8 (2) |
| C11—C12—C13—C14 | 1.2 (3) | C19—Fe1—C18—C17 | 119.4 (3) |
| Fe1—C12—C13—C14 | 59.0 (2) | C13—Fe1—C18—C17 | −32.8 (6) |
| C11—C12—C13—Fe1 | −57.84 (18) | C12—Fe1—C18—C17 | −73.4 (3) |
| C16—Fe1—C13—C14 | 123.0 (2) | C16—C15—C19—C18 | −0.3 (4) |
| C15—Fe1—C13—C14 | 81.5 (2) | Fe1—C15—C19—C18 | −59.8 (2) |
| C11—Fe1—C13—C14 | −82.6 (2) | C16—C15—C19—Fe1 | 59.6 (3) |
| C17—Fe1—C13—C14 | 163.4 (2) | C17—C18—C19—C15 | 0.0 (4) |
| C10—Fe1—C13—C14 | −38.0 (2) | Fe1—C18—C19—C15 | 59.7 (2) |
| C18—Fe1—C13—C14 | −171.0 (4) | C17—C18—C19—Fe1 | −59.7 (2) |
| C19—Fe1—C13—C14 | 50.7 (4) | C16—Fe1—C19—C15 | −37.2 (2) |
| C12—Fe1—C13—C14 | −119.2 (3) | C11—Fe1—C19—C15 | 165.5 (2) |
| C16—Fe1—C13—C12 | −117.8 (2) | C14—Fe1—C19—C15 | 80.0 (2) |
| C15—Fe1—C13—C12 | −159.25 (19) | C17—Fe1—C19—C15 | −81.5 (3) |
| C11—Fe1—C13—C12 | 36.58 (16) | C10—Fe1—C19—C15 | 123.7 (2) |
| C14—Fe1—C13—C12 | 119.2 (3) | C18—Fe1—C19—C15 | −118.9 (3) |
| C17—Fe1—C13—C12 | −77.4 (2) | C13—Fe1—C19—C15 | 44.7 (4) |

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| C10—Fe1—C13—C12 | 81.19 (18) | C12—Fe1—C19—C15 | −161.9 (4) |
| C18—Fe1—C13—C12 | −51.8 (6) | C16—Fe1—C19—C18 | 81.8 (2) |
| C19—Fe1—C13—C12 | 169.9 (3) | C15—Fe1—C19—C18 | 118.9 (3) |
| C12—C13—C14—C10 | −0.5 (4) | C11—Fe1—C19—C18 | −75.5 (3) |
| Fe1—C13—C14—C10 | 59.2 (2) | C14—Fe1—C19—C18 | −161.1 (2) |
| C12—C13—C14—Fe1 | −59.7 (2) | C17—Fe1—C19—C18 | 37.5 (2) |
| C11—C10—C14—C13 | −0.4 (4) | C10—Fe1—C19—C18 | −117.3 (2) |
| C9—C10—C14—C13 | −176.1 (2) | C13—Fe1—C19—C18 | 163.6 (3) |
| Fe1—C10—C14—C13 | −59.8 (2) | C12—Fe1—C19—C18 | −42.9 (6) |
| C11—C10—C14—Fe1 | 59.4 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
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| O1—H1···O2$^{i}$ | 0.82 | 2.04 | 2.841 (3) | 166 |

Symmetry code: (i) *x*+1/2, −*y*+3/2, −*z*.