

(E)-1-Ferrocenyl-3-(2-furyl)prop-2-en-1-one

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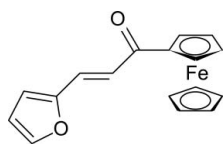
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.023; wR factor = 0.058; data-to-parameter ratio = 16.5.

The title compound, $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{12}\text{H}_9\text{O}_2)]$, exhibits an *E* configuration. In the ferrocene unit, the two cyclopentadienyl rings are almost parallel [dihedral angle = 0.76 (12°)] and the C atoms are in an eclipsed conformation. An intramolecular C—H \cdots O hydrogen bond generates an *S*(5) ring. In the crystal, the molecules are linking into zigzag chains *via* two C—H \cdots O hydrogen-bonding interactions along the *c* axis and neighbouring chains are stabilized by electrostatic interaction forces.

Related literature

For the biological activity of chalcones and chalcone derivatives, see: Liu *et al.* (2003). For the ability of some chalcones to block voltage-dependent potassium channels, see: Yarishkin *et al.* (2008). Replacement of the aromatic group of penicillins and cephalosporins by a ferrocenyl group could improve their antibiotic activity, see: Edwards *et al.* (1975). For our ongoing research in this area, see: Shi *et al.* (2004); Liu, Liu *et al.* (2008). For the synthesis, see: Huang *et al.* (1998). For a related structure, see: Liu, Ye *et al.* (2008) For graph-set notations of ring systems, see: Bernstein *et al.* (1995). For related literature, see: Zhai *et al.* (1999).

**Experimental***Crystal data* $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_{12}\text{H}_9\text{O}_2)]$ $M_r = 306.13$ Orthorhombic, *Pca*2₁ $a = 9.0677$ (13) Å $b = 14.222$ (2) Å $c = 10.4846$ (15) Å $V = 1352.1$ (3) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 1.11$ mm⁻¹ $T = 296$ K

0.28 × 0.25 × 0.22 mm

Data collection

Bruker SMART 1000 CCD

diffractometer

Absorption correction: multi-scan

(SADABS; Bruker, 2002)

 $T_{\min} = 0.746$, $T_{\max} = 0.792$

11058 measured reflections

3012 independent reflections

2772 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.035$ *Refinement* $R[F^2 > 2\sigma(F^2)] = 0.023$ $wR(F^2) = 0.058$ $S = 1.00$

3012 reflections

182 parameters

1 restraint

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Absolute structure: Flack (1983),

1340 Friedel pairs

Flack parameter: 0.012 (14)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C13—H13 \cdots O1	0.93	2.45	2.797 (3)	102
C6—H6 \cdots O1 ¹	0.93	2.56	3.473 (3)	166
C12—H12 \cdots O1 ¹	0.93	2.71	3.576 (4)	155

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

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2265).

References

- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Bruker (2002). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Edwards, E. I., Epton, R. & Marr, G. (1975). *J. Organomet. Chem.* **85**, C23–C25.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Huang, G.-S., Chen, B.-H., Liu, C.-M., Ma, Y.-X. & Liu, Y.-H. (1998). *Transition Met. Chem.* **23**, 589–592.
- Liu, Y.-H., Liu, J.-F., Jian, P.-M. & Liu, X.-L. (2008). *Acta Cryst.* **E64**, m1001–m1002.
- Liu, M., Wilairat, P., Croft, S. L., Tan, A. L. C. & Go, M.-L. (2003). *Bioorg. Med. Chem.* **11**, 2729–2738.
- Liu, Y.-H., Ye, J., Liu, X.-L., Liu, W.-L. & Shi, Y.-C. (2008). *Acta Cryst.* **E64**, m1241.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Shi, Y. C., Yang, H.-M., Song, H.-B. & Liu, Y.-H. (2004). *Polyhedron*, **23**, 1541–1546.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Yarishkin, O. V., Ryu, H. W., Park, J. Y., Yang, M. S., Hong, S. G. & Park, K. H. (2008). *Bioorg. Med. Chem. Lett.* **18**, 137–140.
- Zhai, L., Chen, M., Blom, J., Theander, T. G., Christensen, S. B. & Kharazmi, A. (1999). *Antimicrob. Agents Chemother.* **43**, 793–803.

supplementary materials

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(*E*)-1-Ferrocenyl-3-(2-furyl)prop-2-en-1-one

Y.-H. Liu and R. Guo

Comment

Chalcone and its derivatives, as a natural produce, have shown strong antibacterial, antifungal, antitumor and anti-inflammatory properties (Liu *et al.*, 2003). Some chalcones demonstrated the ability to block voltage-dependent potassium channels (Yarishkin *et al.*, 2008). It has been demonstrated that the replacement of the aromatic group by the ferrocenyl moiety in penicillins and cephalosporins could improve their antibiotic activity (Edwards *et al.*, 1975). As on going research (Liu & Liu *et al.*, 2008; Shi *et al.*, 2004), we report herein the structure of the title compound.

The molecule of the title compound exists in the most stable configuration of (*E*)-isomer (Fig. 1). All of the C and O atoms are sp^2 -hybrid resulting in two large conjugated systems: one is formed by C1-C5 atoms and the other by the rest of the atoms. There is an intra-molecular hydrogen-bond C13–H13 \cdots O1 resulting in a five membered ring, $S(5)$ in graph set notation (Bernstein *et al.*, 1995). The atoms O1/C11/C12/C13 are essentially planar and their mean-plane lies at 3.10 (14) and 16.35 (13) °, respectively, with the mean-planes of the furyl ring and the substituted cyclopentadienyl ring. In the ferrocene moiety, the Cps plane and Cp (the unsubstituted cyclopentadienyl ring) plane are almost parallel and the C atoms of Cp and Cps are in the eclipsed conformation. The Fe atom is slightly near the Cps plane as the distances Fe–Cgs and Fe–Cg are 1.6464 (9) and 1.6574 (10) Å, respectively, where Cgs and Cg are the centroids of Cps and Cp, respectively. The Cgs–Fe–Cg angle is 179.02 (5)°. The molecular dimensions agree very well with the corresponding dimensions reported for the crystal structure of a similar compound (Liu & Ye *et al.*, 2008).

In the crystal structure, inter-molecular hydrogen-bonds of the type C—H \cdots O, along the *c* axis, generate a $R_2^1(7)$ motif (Bernstein *et al.*, 1995), linking the adjacent molecules into a zig-zag chain (Fig. 2, Tab. 1). Further more, the chain and its neighboring inverse parallel chains are stabilized by electrostatic interaction forces.

Experimental

The title compound was synthesized according to the literature procedure (Huang *et al.*, 1998). An aqueous solution of potassium hydroxide (5%, 5 ml) was added slowly with stirring to a mixture of 2-furanylaldehyde (4.0 g, 0.043 mol) and acetylferrocene (0.98 g, 0.043 mol) in ethanol (20 ml) in ice bath. The resulting mixture was stirred at room temperature for 4 h. The dark-red precipitated solid was filtered off, washed with water, dried and recrystallized from 95% ethanol (yield, 83%; M.P. 429.5-430.8 K. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a solution of the solid in dichloromethane/ ether (4:1 v/v) at room temperature over a period of 6 d.

Refinement

After their location in a difference map, all H atoms were fixed geometrically at ideal positions and allowed to ride on the parent C atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. An absolute structure was determined using anomalous dispersion effects employing 1353 Friedel pairs which were not merged.

Figures

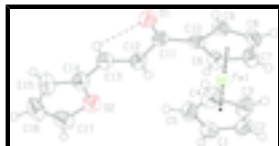


Fig. 1. The molecular structure of the title compound, showing 50% probability ellipsoids. The C–H···O intra-molecular hydrogen bond is shown as dashed lines.

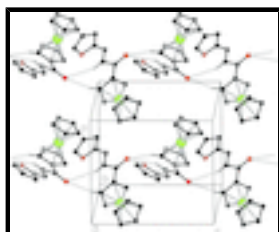


Fig. 2. Unit cell packing of the title compound, showing the inter-molecular hydrogen bonds C–H···O as dashed lines. For the sake of clarity, H atoms not involved in hydrogen bonding have been omitted.

(*E*)-1-Ferrocenyl-3-(2-furyl)prop-2-en-1-one

Crystal data

[Fe(C₅H₅)(C₁₂H₉O₂)]

$M_r = 306.13$

Orthorhombic, *Pca*2₁

Hall symbol: P 2c -2ac

$a = 9.0677$ (13) Å

$b = 14.222$ (2) Å

$c = 10.4846$ (15) Å

$V = 1352.1$ (3) Å³

$Z = 4$

$F(000) = 632$

$D_x = 1.504$ Mg m⁻³

Melting point: 429.5 K

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

Cell parameters from 6056 reflections

$\theta = 2.7$ – 27.4°

$\mu = 1.11$ mm⁻¹

$T = 296$ K

Prism, orange

$0.28 \times 0.25 \times 0.22$ mm

Data collection

Bruker SMART 1000 CCD
diffractometer

Radiation source: fine-focus sealed tube
graphite

ϕ and ω scans

Absorption correction: multi-scan
(SADABS; Bruker, 2002)

$T_{\min} = 0.746$, $T_{\max} = 0.792$

11058 measured reflections

3012 independent reflections

2772 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$

$\theta_{\max} = 27.7^\circ$, $\theta_{\min} = 2.7^\circ$

$h = -11 \rightarrow 11$

$k = -18 \rightarrow 16$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.023$

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0253P)^2 + 0.1177P]$

$wR(F^2) = 0.058$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\max} = 0.001$
3012 reflections	$\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$
182 parameters	$\Delta\rho_{\min} = -0.19 \text{ e } \text{\AA}^{-3}$
1 restraint	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0184 (11) Absolute structure: Flack (1983), 1340 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.012 (14)

Special details

Experimental. Analysis found (calculated) for $C_{17}H_{14}FeO_2$ (%): C 66.61 (66.70), H 4.56 (4.61).

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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	-0.04553 (2)	0.652980 (14)	0.19388 (4)	0.03343 (8)
O1	0.35975 (15)	0.71855 (11)	0.24502 (15)	0.0524 (4)
O2	0.28635 (15)	0.93776 (10)	-0.13390 (15)	0.0525 (3)
C1	-0.1739 (2)	0.76594 (14)	0.1431 (2)	0.0523 (5)
H1	-0.1789	0.7934	0.0627	0.063*
C2	-0.26341 (18)	0.69146 (14)	0.1893 (3)	0.0522 (4)
H2	-0.3381	0.6615	0.1440	0.063*
C3	-0.2206 (2)	0.67061 (16)	0.3142 (2)	0.0550 (6)
H3	-0.2613	0.6243	0.3661	0.066*
C4	-0.1041 (2)	0.73260 (17)	0.3481 (2)	0.0582 (6)
H4	-0.0554	0.7344	0.4261	0.070*
C5	-0.0756 (2)	0.79058 (15)	0.2428 (3)	0.0555 (6)
H5	-0.0042	0.8374	0.2390	0.067*
C6	0.0731 (2)	0.61272 (14)	0.03780 (19)	0.0430 (4)
H6	0.0722	0.6417	-0.0417	0.052*
C7	-0.0200 (2)	0.53753 (14)	0.0779 (2)	0.0484 (5)
H7	-0.0924	0.5087	0.0287	0.058*
C8	0.0167 (2)	0.51418 (13)	0.2055 (3)	0.0493 (5)
H8	-0.0278	0.4675	0.2543	0.059*
C9	0.13284 (19)	0.57416 (13)	0.2463 (2)	0.0455 (4)
H9	0.1776	0.5736	0.3261	0.055*

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C10	0.16853 (19)	0.63550 (13)	0.14257 (19)	0.0385 (4)
C11	0.27507 (18)	0.71373 (13)	0.15362 (18)	0.0386 (4)
C12	0.2747 (2)	0.78616 (13)	0.05229 (18)	0.0398 (4)
H12	0.2132	0.7793	-0.0181	0.048*
C13	0.3620 (2)	0.86111 (13)	0.06132 (19)	0.0418 (4)
H13	0.4231	0.8638	0.1325	0.050*
C14	0.3723 (2)	0.93831 (14)	-0.02664 (19)	0.0436 (4)
C15	0.4527 (2)	1.01887 (16)	-0.0245 (2)	0.0568 (6)
H15	0.5206	1.0363	0.0376	0.068*
C17	0.3148 (3)	1.02013 (17)	-0.1960 (3)	0.0614 (6)
H16	0.2704	1.0383	-0.2720	0.074*
C16	0.4146 (3)	1.07107 (16)	-0.1333 (3)	0.0630 (6)
H17	0.4516	1.1295	-0.1569	0.076*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.03501 (11)	0.03456 (13)	0.03073 (12)	-0.00320 (8)	0.00069 (13)	-0.00016 (13)
O1	0.0483 (7)	0.0608 (9)	0.0481 (8)	-0.0051 (6)	-0.0080 (6)	0.0125 (7)
O2	0.0544 (8)	0.0487 (8)	0.0545 (9)	-0.0015 (6)	-0.0052 (7)	0.0061 (7)
C1	0.0495 (11)	0.0416 (11)	0.0659 (14)	0.0076 (8)	-0.0004 (9)	0.0000 (9)
C2	0.0351 (7)	0.0549 (10)	0.0666 (13)	-0.0006 (7)	-0.0031 (11)	-0.0056 (15)
C3	0.0449 (10)	0.0650 (14)	0.0551 (14)	-0.0073 (9)	0.0148 (9)	-0.0063 (11)
C4	0.0514 (11)	0.0724 (15)	0.0507 (13)	-0.0033 (10)	0.0060 (9)	-0.0240 (12)
C5	0.0476 (10)	0.0414 (11)	0.0775 (17)	-0.0027 (8)	0.0095 (10)	-0.0170 (10)
C6	0.0554 (10)	0.0400 (10)	0.0336 (10)	0.0012 (8)	0.0074 (8)	-0.0022 (8)
C7	0.0596 (11)	0.0368 (10)	0.0487 (12)	-0.0034 (9)	0.0028 (9)	-0.0078 (9)
C8	0.0535 (9)	0.0335 (8)	0.0611 (14)	-0.0005 (7)	0.0061 (12)	0.0097 (12)
C9	0.0433 (9)	0.0439 (11)	0.0493 (11)	0.0046 (8)	0.0006 (8)	0.0142 (8)
C10	0.0380 (8)	0.0394 (9)	0.0380 (9)	0.0069 (7)	0.0059 (7)	0.0036 (7)
C11	0.0328 (8)	0.0436 (10)	0.0394 (10)	0.0044 (7)	0.0058 (7)	0.0046 (7)
C12	0.0391 (9)	0.0454 (10)	0.0348 (10)	-0.0003 (8)	0.0023 (7)	0.0036 (8)
C13	0.0436 (9)	0.0451 (10)	0.0365 (10)	-0.0010 (8)	0.0045 (7)	0.0005 (8)
C14	0.0460 (10)	0.0441 (11)	0.0408 (10)	-0.0008 (8)	0.0072 (8)	-0.0030 (8)
C15	0.0697 (14)	0.0522 (13)	0.0486 (13)	-0.0186 (10)	0.0019 (9)	-0.0009 (10)
C17	0.0744 (14)	0.0521 (13)	0.0578 (15)	0.0124 (11)	0.0043 (12)	0.0136 (10)
C16	0.0848 (16)	0.0428 (12)	0.0614 (15)	-0.0070 (12)	0.0217 (13)	0.0049 (11)

Geometric parameters (\AA , $^\circ$)

Fe1—C10	2.0295 (18)	C5—H5	0.9300
Fe1—C6	2.0404 (19)	C6—C7	1.426 (3)
Fe1—C5	2.041 (2)	C6—C10	1.435 (3)
Fe1—C9	2.0431 (18)	C6—H6	0.9300
Fe1—C3	2.044 (2)	C7—C8	1.418 (4)
Fe1—C4	2.044 (2)	C7—H7	0.9300
Fe1—C2	2.0506 (17)	C8—C9	1.421 (3)
Fe1—C1	2.054 (2)	C8—H8	0.9300
Fe1—C7	2.056 (2)	C9—C10	1.431 (3)

Fe1—C8	2.0566 (18)	C9—H9	0.9300
O1—C11	1.230 (2)	C10—C11	1.478 (3)
O2—C17	1.365 (3)	C11—C12	1.480 (3)
O2—C14	1.369 (2)	C12—C13	1.331 (3)
C1—C5	1.418 (3)	C12—H12	0.9300
C1—C2	1.419 (3)	C13—C14	1.437 (3)
C1—H1	0.9300	C13—H13	0.9300
C2—C3	1.398 (4)	C14—C15	1.358 (3)
C2—H2	0.9300	C15—C16	1.404 (4)
C3—C4	1.421 (3)	C15—H15	0.9300
C3—H3	0.9300	C17—C16	1.332 (4)
C4—C5	1.402 (4)	C17—H16	0.9300
C4—H4	0.9300	C16—H17	0.9300
C10—Fe1—C6	41.30 (8)	C5—C4—C3	107.8 (2)
C10—Fe1—C5	108.18 (8)	C5—C4—Fe1	69.82 (13)
C6—Fe1—C5	122.75 (9)	C3—C4—Fe1	69.63 (12)
C10—Fe1—C9	41.14 (7)	C5—C4—H4	126.1
C6—Fe1—C9	69.16 (9)	C3—C4—H4	126.1
C5—Fe1—C9	124.36 (9)	Fe1—C4—H4	126.0
C10—Fe1—C3	157.20 (9)	C4—C5—C1	108.63 (19)
C6—Fe1—C3	159.93 (9)	C4—C5—Fe1	70.04 (12)
C5—Fe1—C3	67.88 (9)	C1—C5—Fe1	70.24 (12)
C9—Fe1—C3	121.09 (9)	C4—C5—H5	125.7
C10—Fe1—C4	121.74 (9)	C1—C5—H5	125.7
C6—Fe1—C4	157.94 (9)	Fe1—C5—H5	125.6
C5—Fe1—C4	40.14 (11)	C7—C6—C10	107.50 (18)
C9—Fe1—C4	107.27 (10)	C7—C6—Fe1	70.23 (11)
C3—Fe1—C4	40.70 (9)	C10—C6—Fe1	68.95 (11)
C10—Fe1—C2	161.43 (10)	C7—C6—H6	126.3
C6—Fe1—C2	124.34 (11)	C10—C6—H6	126.3
C5—Fe1—C2	67.74 (8)	Fe1—C6—H6	126.1
C9—Fe1—C2	156.26 (9)	C8—C7—C6	108.35 (18)
C3—Fe1—C2	39.92 (11)	C8—C7—Fe1	69.85 (12)
C4—Fe1—C2	67.69 (10)	C6—C7—Fe1	69.03 (11)
C10—Fe1—C1	124.69 (8)	C8—C7—H7	125.8
C6—Fe1—C1	108.09 (9)	C6—C7—H7	125.8
C5—Fe1—C1	40.50 (9)	Fe1—C7—H7	126.9
C9—Fe1—C1	161.34 (8)	C7—C8—C9	108.49 (18)
C3—Fe1—C1	67.89 (10)	C7—C8—Fe1	69.82 (11)
C4—Fe1—C1	67.95 (10)	C9—C8—Fe1	69.21 (10)
C2—Fe1—C1	40.46 (8)	C7—C8—H8	125.8
C10—Fe1—C7	68.76 (8)	C9—C8—H8	125.8
C6—Fe1—C7	40.74 (8)	Fe1—C8—H8	126.8
C5—Fe1—C7	158.29 (10)	C8—C9—C10	107.7 (2)
C9—Fe1—C7	68.39 (9)	C8—C9—Fe1	70.23 (10)
C3—Fe1—C7	123.40 (9)	C10—C9—Fe1	68.92 (10)
C4—Fe1—C7	159.94 (10)	C8—C9—H9	126.1
C2—Fe1—C7	107.92 (9)	C10—C9—H9	126.1
C1—Fe1—C7	122.34 (9)	Fe1—C9—H9	126.3

supplementary materials

C10—Fe1—C8	68.64 (8)	C9—C10—C6	107.91 (16)
C6—Fe1—C8	68.50 (10)	C9—C10—C11	123.17 (18)
C5—Fe1—C8	160.39 (11)	C6—C10—C11	128.60 (17)
C9—Fe1—C8	40.57 (8)	C9—C10—Fe1	69.94 (10)
C3—Fe1—C8	107.12 (10)	C6—C10—Fe1	69.76 (10)
C4—Fe1—C8	123.79 (12)	C11—C10—Fe1	120.80 (13)
C2—Fe1—C8	121.45 (8)	O1—C11—C10	120.74 (17)
C1—Fe1—C8	157.13 (10)	O1—C11—C12	121.46 (17)
C7—Fe1—C8	40.33 (11)	C10—C11—C12	117.79 (16)
C17—O2—C14	106.22 (17)	C13—C12—C11	120.34 (18)
C5—C1—C2	107.0 (2)	C13—C12—H12	119.8
C5—C1—Fe1	69.26 (12)	C11—C12—H12	119.8
C2—C1—Fe1	69.63 (11)	C12—C13—C14	127.24 (19)
C5—C1—H1	126.5	C12—C13—H13	116.4
C2—C1—H1	126.5	C14—C13—H13	116.4
Fe1—C1—H1	126.2	C15—C14—O2	108.90 (19)
C3—C2—C1	108.6 (2)	C15—C14—C13	132.0 (2)
C3—C2—Fe1	69.77 (11)	O2—C14—C13	119.06 (17)
C1—C2—Fe1	69.91 (10)	C14—C15—C16	107.5 (2)
C3—C2—H2	125.7	C14—C15—H15	126.3
C1—C2—H2	125.7	C16—C15—H15	126.3
Fe1—C2—H2	126.2	C16—C17—O2	111.1 (2)
C2—C3—C4	108.0 (2)	C16—C17—H16	124.4
C2—C3—Fe1	70.31 (12)	O2—C17—H16	124.4
C4—C3—Fe1	69.67 (12)	C17—C16—C15	106.3 (2)
C2—C3—H3	126.0	C17—C16—H17	126.9
C4—C3—H3	126.0	C15—C16—H17	126.9
Fe1—C3—H3	125.6		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C13—H13 \cdots O1	0.93	2.45	2.797 (3)	102
C6—H6 \cdots O1 ⁱ	0.93	2.56	3.473 (3)	166
C12—H12 \cdots O1 ⁱ	0.93	2.71	3.576 (4)	155

Symmetry codes: (i) $-x+1/2, y, z-1/2$.

Fig. 1

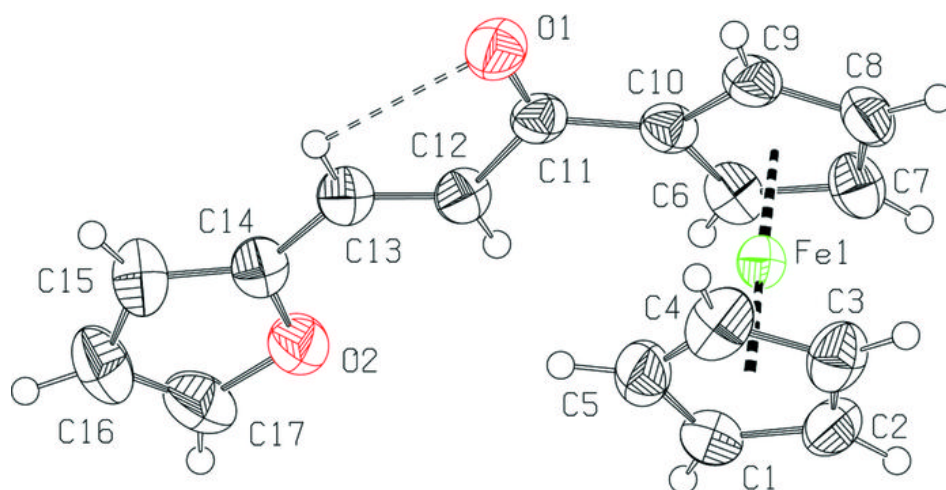


Fig. 2

