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# 1-Ferrocenyl-3-(4-*n*-octoxylphenyl)-propane-1,3-dione

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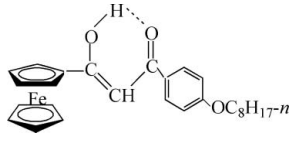
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.040; $wR$ factor = 0.103; data-to-parameter ratio = 17.8.

The title compound, $[Fe(C_5H_5)(C_{22}H_{27}O_3)]$, which forms an extended conjugated system and appears in the enol form, is mainly stabilized by an intramolecular hydrogen bond. The Fe—C bond distances are nearly equal with a mean value of 2.0312 Å. The two cyclopentadienyl rings are almost parallel to each other, as shown by the dihedral angle of 0.97 (17)°. In the structure, ferrocenyl is the more powerful electron-donating group, with the result that the carbonyl group substituted on the benzene ring has the enol form.

## Related literature

For related literature, see: Kato (2002); Koizumi *et al.* (2002); Plazuk *et al.* (2001); Zhang *et al.* (2006); Gin *et al.* (2001); Kato *et al.* (2006); Oriol & Serrano (2005); Shi *et al.* (2006); Trzaska *et al.* (1999).




## Experimental

### Crystal data

$[Fe(C_5H_5)(C_{22}H_{27}O_3)]$
$M_r$ = 460.38
Monoclinic, $P2_1/c$
$a$ = 18.5985 (14) Å
$b$ = 10.5710 (8) Å
$c$ = 12.0814 (10) Å
$\beta$ = 95.1050 (10)°
$V$ = 2365.8 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.66 mm$^{-1}$
$T$ = 293 (2) K
0.49 × 0.42 × 0.24 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.752, $T_{max}$ = 1.000
(expected range = 0.642–0.854)
13567 measured reflections
5151 independent reflections
3981 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.056

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.103
$S$ = 0.96
5151 reflections
290 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.34 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2$A$···O1 | 0.852 (17) | 1.72 (2) | 2.499 (2) | 151 (3) |

Data collection: *SMART* (Bruker 1997); cell refinement: *SAINT* (Bruker 1997); data reduction: *SHELXTL* (Sheldrick, 1997*a*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*b*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The reflection data were collected at the Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences. This work was financially supported by the Natural Science Foundation of Inner Mongolia, China (grant No. 200308020103).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SF3061).

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# supplementary materials

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# 1-Ferrocenyl-3-(4-*n*-octoxylphenyl)propane-1,3-dione

**Y. Shang, B. Li, R. Hu, Y. Su and Q. Tang**

## Comment

There has been a growing interest in functional liquid crystal materials (Kato,2002; Kato *et al.*, 2006; Gin *et al.*, 2001). For instance, incorporation of metal atoms into liquid crystalline materals (metallmesoges) provides new opportunities in materials science through tuning of anisotropic optical, electronic, and magnetic properties (Oriol & Serrano, 2005; Trzaska *et al.*, 1999). Mixed ferrocene/beta-diketones mesogens have therefore attracted considerable attention for their potential redox switching activity and stability (Plazuk *et al.*, 2001; Koizumi *et al.*, 2002). In view of theapplications as the ligand of transition metal complexes which could be shown liquid crystalline properties, we have designed and synthesized the title compound,(I) (Figure. 1), derived by the condensation of actylferrocene and methyl 4-octanoxy benzonate.

From the crystal structure data, it is indicated that both cyclopentadienyl (Cp) groups of (I) are coplanar with the largest torsion angle 0.3 (3) ° between the two endocyclic C—C bonds for C2—C3—C4—C5 and the largest deviation of C atom of −0.0017(0.0014) for C3. The two Cp rings are almost parallel to each other as shown by the dihedral angle of 0.97 (0.17)°. The distances between Fe atom and two Cp planes are 1.6386 (0.0008) and 1.6436 (0.0010) Å,respectively and the distance between the two Cp rings is 3.2822 Å. The Fe—C bond distances are nearly equidistant and possess a mean value of 2.0312 Å and the mean distance of C—C bonds within Cp rings is 1.407 Å, whereas C6—C10 of 1.423 (2) Å and C9—C10 of 1.432 (2) Å are slightly longer due to the effect of substituted group. The mean value of bond angles of C—Fe—C is 40.53° and of Fe—C—C is 69.85° when the two carbon atoms are adjacent within the Cp rings. The bond angles of adjacent C—C—C in the same cyclopentadienyl ring have a mean value of 108.0°. The data above accord with the literature reported (Glidewell *et al.*, 1996; Zhang *et al.*, 2006). The bond length of C11—C12 (1.398 (3) Å) and C12—C13 (1.387 (2) Å) is shorter than the normal value of single C—C bond (1.54 Å) but close to the normal carbon-carbon double bond (1.34 Å) becaused of beta-diketone enolization. Enolization of the title compound (I) can also account for the bond length of O1—C11 and O2—C13 which is 1.285 (2) and 1.295 (2) Å respectively and remarkably shorter than the normal value of single O—C bond (1.42 Å) but a little longer than the normal C═O double bond (1.22 Å). Bond length O3—C17 of 1.395 (2) Å with partially double bonded properties results from conjugation of benzene ring and is shorter than the normal single O—C bond such as O3—C20 of 1.432 (2) Å. The ferrocenyl is a more powerful electron-donating group, resulting that the carbonyl group substituted on benzene ring favors the form of enol as shown in scheme below, which is also demonstrated by the shorter bond length of C12—C13 than that of C11—C12. The enol form of the beta-diketone is stabilized by an intramolecular hydrogen bonding (O1···H2A—O2: bond length 1.72 (2) Å, bond angle 151 (3) °, O2—H2A bond length 0.852 (17) Å, symmetry codes: (−*x*,*y* + 1/2,-*z* + 1/2). The bond angles around C11, C12 and C13 all averaging to 120° respectively demonstrated these atoms of $sp^2$ hybridization.

## Experimental

The title compound was synthesized by dropwise additon of methyl 4-octanoxy benzonate (4 mmol) to a 25 ml dimethoxy-ethane solution of NaH (33 mmol) and acetylferrocene (4 mmol) under $N_2$. After the mixture were kept refluxing for 4 h, the solvent was evaporated, the remaining product was washed by 5% KOH solution for several times then extracted

with benzene, the resulting product was purified by column chromatography (silica gel,100—200 meshes, eluant petroleum ether). The solid residue was recrystallized using petroleum ether by slow evaporation to afford dark red crystals (yield 76%, m.p.353 K). 1HNMR ($CDCl_3$, 500 MHz): delta 6.99 (m, 4H, Ar—H), 6.35 (s, 2H, $COCH_2CO$), 4.91—4.55 (m, 4H, $C_5H_4$), 4.24 (s, 5H, $C_5H_5$), 1.85—1.32 (m, 14 H, $O(CH_2)_7$), 0.92 (t, 3H, $CH_3$).

All H atoms were included in calculated positions as riding atoms, with C—H distance of 0.93 Å for aromatic H atoms, 0.893 Å for methine H atoms, 0.97 Å for methylene H atoms and 0.96 Å for the methyl H atom.

## Figures

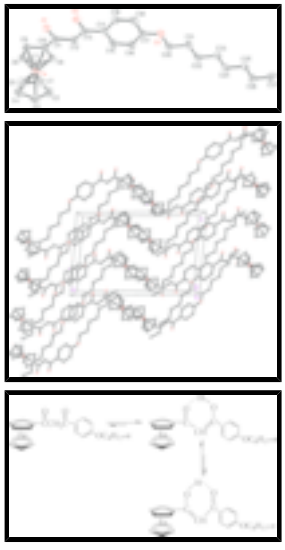

Figure. 1. The X-ray crystal structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering s cheme. H atoms have been omitted for clarity. Figure. 2. A packing diagram for (I), viewed along the *c* axis. The *a* axis is to the right and the *b* axis is upwards.

## 1-Ferrocenyl-3-(4-n-octoxylphenyl)propane-1,3-dione

*Crystal data*

| | |
|---|---|
| $[Fe(C_5H_5)(C_{22}H_{27}O_3)]$ | $D_x = 1.293$ Mg m$^{-3}$ |
| $M_r = 460.38$ | Melting point: 353 K |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| $a = 18.5985$ (14) Å | Cell parameters from 5300 reflections |
| $b = 10.5710$ (8) Å | $\theta = 4.4$–$54.5^o$ |
| $c = 12.0814$ (10) Å | $\mu = 0.66$ mm$^{-1}$ |
| $\beta = 95.1050$ (10)º | $T = 293$ (2) K |
| $V = 2365.8$ (3) Å$^3$ | Prismatic, red |
| $Z = 4$ | 0.49 × 0.42 × 0.24 mm |
| $F_{000} = 976$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 5151 independent reflections |
| Radiation source: fine-focus sealed tube | 3981 reflections with $I > 2\sigma(I)$ |

| | |
|---|---|
| Monochromator: graphite | $R_{int}$ = 0.056 |
| $T$ = 293(2) K | $\theta_{max}$ = 27.0º |
| phi and ω scans | $\theta_{min}$ = 2.2º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −23→20 |
| $T_{min}$ = 0.752, $T_{max}$ = 1.000 | $k$ = −10→13 |
| 13567 measured reflections | $l$ = −15→14 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.040 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.103 | $w = 1/[\sigma^2(F_o^2) + (0.0587P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 0.96 | $(\Delta/\sigma)_{max}$ = 0.013 |
| 5151 reflections | $\Delta\rho_{max}$ = 0.44 e Å$^{-3}$ |
| 290 parameters | $\Delta\rho_{min}$ = −0.34 e Å$^{-3}$ |
| 2 restraints | Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.0016 (5) |

*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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Fe | 0.410173 (12) | 0.40073 (2) | 0.66175 (2) | 0.04243 (11) |
| O1 | 0.26966 (7) | 0.25316 (14) | 0.45703 (11) | 0.0625 (4) |
| O2 | 0.16093 (8) | 0.13125 (15) | 0.50208 (12) | 0.0596 (4) |
| O3 | −0.06702 (8) | 0.08529 (13) | 0.85417 (12) | 0.0643 (4) |
| C1 | 0.41834 (12) | 0.2181 (2) | 0.7121 (2) | 0.0738 (7) |
| H1 | 0.3847 | 0.1548 | 0.6937 | 0.089* |
| C2 | 0.41979 (13) | 0.2987 (2) | 0.80485 (19) | 0.0713 (6) |
| H2 | 0.3872 | 0.2979 | 0.8590 | 0.086* |

| | | | | |
|---|---|---|---|---|
| C3 | 0.47802 (15) | 0.3793 (2) | 0.8014 (2) | 0.0769 (7) |
| H3 | 0.4913 | 0.4424 | 0.8529 | 0.092* |
| C4 | 0.51349 (12) | 0.3502 (3) | 0.7082 (2) | 0.0770 (7) |
| H4 | 0.5546 | 0.3905 | 0.6872 | 0.092* |
| C5 | 0.47771 (13) | 0.2510 (2) | 0.6515 (2) | 0.0719 (6) |
| H5 | 0.4902 | 0.2134 | 0.5863 | 0.086* |
| C6 | 0.31896 (9) | 0.50533 (17) | 0.66238 (16) | 0.0489 (4) |
| H6 | 0.2874 | 0.5058 | 0.7179 | 0.059* |
| C7 | 0.37895 (11) | 0.58600 (16) | 0.65660 (18) | 0.0535 (5) |
| H7 | 0.3938 | 0.6487 | 0.7076 | 0.064* |
| C8 | 0.41245 (10) | 0.55505 (17) | 0.56015 (17) | 0.0529 (5) |
| H8 | 0.4533 | 0.5940 | 0.5366 | 0.063* |
| C9 | 0.37379 (10) | 0.45521 (18) | 0.50528 (15) | 0.0496 (4) |
| H9 | 0.3846 | 0.4169 | 0.4395 | 0.060* |
| C10 | 0.31494 (9) | 0.42315 (16) | 0.56879 (16) | 0.0445 (4) |
| C11 | 0.26385 (9) | 0.31945 (17) | 0.54492 (15) | 0.0460 (4) |
| C12 | 0.20941 (10) | 0.29419 (18) | 0.61446 (16) | 0.0494 (4) |
| C13 | 0.15841 (9) | 0.20017 (17) | 0.59023 (15) | 0.0452 (4) |
| C14 | 0.09937 (9) | 0.17412 (16) | 0.66001 (15) | 0.0459 (4) |
| C15 | 0.09550 (10) | 0.2317 (2) | 0.76240 (18) | 0.0601 (5) |
| H15 | 0.1308 | 0.2902 | 0.7868 | 0.072* |
| C16 | 0.04136 (10) | 0.2051 (2) | 0.82892 (18) | 0.0611 (5) |
| H16 | 0.0406 | 0.2445 | 0.8976 | 0.073* |
| C17 | −0.01206 (10) | 0.11943 (18) | 0.79344 (17) | 0.0521 (5) |
| C18 | −0.00993 (11) | 0.0630 (2) | 0.69056 (18) | 0.0628 (5) |
| H18 | −0.0462 | 0.0067 | 0.6652 | 0.075* |
| C19 | 0.04489 (11) | 0.08889 (18) | 0.62566 (17) | 0.0565 (5) |
| H19 | 0.0458 | 0.0488 | 0.5573 | 0.068* |
| C20 | −0.06966 (10) | 0.1404 (2) | 0.96201 (18) | 0.0586 (5) |
| H20A | −0.0743 | 0.2316 | 0.9556 | 0.070* |
| H20B | −0.0255 | 0.1215 | 1.0080 | 0.070* |
| C21 | −0.13316 (11) | 0.08680 (19) | 1.01395 (18) | 0.0590 (5) |
| H21A | −0.1280 | −0.0043 | 1.0194 | 0.071* |
| H21B | −0.1767 | 0.1046 | 0.9663 | 0.071* |
| C22 | −0.14099 (10) | 0.1403 (2) | 1.12839 (17) | 0.0599 (5) |
| H22A | −0.1444 | 0.2317 | 1.1231 | 0.072* |
| H22B | −0.0980 | 0.1200 | 1.1765 | 0.072* |
| C23 | −0.20655 (11) | 0.09033 (19) | 1.18099 (17) | 0.0577 (5) |
| H23A | −0.2496 | 0.1132 | 1.1341 | 0.069* |
| H23B | −0.2040 | −0.0013 | 1.1836 | 0.069* |
| C24 | −0.21352 (11) | 0.1393 (2) | 1.29670 (18) | 0.0608 (5) |
| H24A | −0.2160 | 0.2309 | 1.2939 | 0.073* |
| H24B | −0.1703 | 0.1165 | 1.3434 | 0.073* |
| C25 | −0.27851 (11) | 0.09053 (19) | 1.35034 (18) | 0.0595 (5) |
| H25A | −0.3219 | 0.1165 | 1.3056 | 0.071* |
| H25B | −0.2772 | −0.0012 | 1.3506 | 0.071* |
| C26 | −0.28289 (13) | 0.1364 (2) | 1.46786 (19) | 0.0704 (6) |
| H26A | −0.2403 | 0.1079 | 1.5133 | 0.085* |
| H26B | −0.2826 | 0.2281 | 1.4681 | 0.085* |

| | | | | |
|---|---|---|---|---|
| C27 | −0.34914 (17) | 0.0907 (3) | 1.5191 (2) | 0.1007 (10) |
| H27A | −0.3916 | 0.1191 | 1.4751 | 0.121* |
| H27B | −0.3491 | 0.1239 | 1.5931 | 0.121* |
| H27C | −0.3489 | −0.0001 | 1.5220 | 0.121* |
| H12 | 0.2083 (9) | 0.3413 (16) | 0.6756 (13) | 0.046 (5)* |
| H2A | 0.1963 (12) | 0.156 (3) | 0.468 (2) | 0.107 (11)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Fe | 0.03781 (16) | 0.04017 (16) | 0.04925 (18) | 0.00032 (10) | 0.00359 (11) | 0.00728 (11) |
| O1 | 0.0600 (8) | 0.0718 (9) | 0.0564 (9) | −0.0068 (7) | 0.0085 (7) | −0.0158 (7) |
| O2 | 0.0574 (9) | 0.0673 (9) | 0.0533 (9) | −0.0097 (7) | 0.0001 (7) | −0.0133 (7) |
| O3 | 0.0587 (8) | 0.0717 (10) | 0.0635 (9) | −0.0214 (7) | 0.0107 (7) | −0.0110 (7) |
| C1 | 0.0664 (14) | 0.0423 (11) | 0.109 (2) | −0.0009 (10) | −0.0108 (13) | 0.0249 (12) |
| C2 | 0.0807 (15) | 0.0706 (15) | 0.0643 (15) | 0.0110 (12) | 0.0154 (12) | 0.0283 (12) |
| C3 | 0.0842 (17) | 0.0758 (16) | 0.0648 (16) | −0.0036 (13) | −0.0255 (14) | 0.0157 (12) |
| C4 | 0.0416 (11) | 0.0894 (18) | 0.098 (2) | 0.0047 (12) | −0.0060 (12) | 0.0356 (15) |
| C5 | 0.0711 (14) | 0.0673 (14) | 0.0782 (16) | 0.0328 (12) | 0.0119 (12) | 0.0119 (12) |
| C6 | 0.0426 (9) | 0.0457 (10) | 0.0590 (12) | 0.0043 (8) | 0.0081 (8) | −0.0020 (9) |
| C7 | 0.0538 (11) | 0.0381 (10) | 0.0677 (13) | −0.0001 (8) | 0.0008 (9) | −0.0013 (9) |
| C8 | 0.0534 (11) | 0.0426 (10) | 0.0633 (13) | −0.0022 (8) | 0.0091 (9) | 0.0143 (9) |
| C9 | 0.0539 (11) | 0.0499 (11) | 0.0454 (10) | 0.0044 (9) | 0.0058 (8) | 0.0081 (8) |
| C10 | 0.0384 (9) | 0.0440 (10) | 0.0506 (11) | 0.0050 (7) | 0.0019 (8) | 0.0019 (8) |
| C11 | 0.0406 (9) | 0.0468 (10) | 0.0491 (11) | 0.0056 (7) | −0.0042 (8) | −0.0001 (8) |
| C12 | 0.0480 (10) | 0.0499 (11) | 0.0502 (11) | −0.0035 (8) | 0.0026 (8) | −0.0116 (9) |
| C13 | 0.0416 (9) | 0.0475 (10) | 0.0451 (10) | 0.0042 (8) | −0.0051 (7) | 0.0004 (8) |
| C14 | 0.0419 (9) | 0.0433 (10) | 0.0507 (11) | −0.0017 (7) | −0.0065 (8) | 0.0000 (8) |
| C15 | 0.0523 (11) | 0.0621 (12) | 0.0659 (13) | −0.0192 (9) | 0.0056 (9) | −0.0181 (10) |
| C16 | 0.0563 (12) | 0.0658 (13) | 0.0618 (13) | −0.0163 (10) | 0.0090 (10) | −0.0189 (10) |
| C17 | 0.0462 (10) | 0.0512 (11) | 0.0582 (12) | −0.0075 (8) | 0.0008 (9) | −0.0013 (9) |
| C18 | 0.0602 (12) | 0.0643 (13) | 0.0631 (13) | −0.0228 (10) | 0.0005 (10) | −0.0095 (10) |
| C19 | 0.0570 (12) | 0.0604 (13) | 0.0511 (12) | −0.0130 (9) | −0.0006 (9) | −0.0089 (9) |
| C20 | 0.0519 (11) | 0.0627 (12) | 0.0612 (13) | −0.0083 (10) | 0.0047 (9) | −0.0044 (10) |
| C21 | 0.0532 (11) | 0.0613 (13) | 0.0625 (13) | −0.0097 (9) | 0.0048 (10) | −0.0002 (10) |
| C22 | 0.0506 (11) | 0.0634 (12) | 0.0646 (14) | −0.0076 (9) | −0.0007 (10) | −0.0024 (10) |
| C23 | 0.0544 (11) | 0.0598 (13) | 0.0586 (13) | −0.0056 (9) | 0.0024 (10) | 0.0000 (9) |
| C24 | 0.0553 (12) | 0.0619 (12) | 0.0645 (14) | −0.0042 (10) | 0.0018 (10) | −0.0034 (10) |
| C25 | 0.0542 (11) | 0.0638 (13) | 0.0598 (13) | 0.0002 (9) | 0.0013 (10) | 0.0015 (10) |
| C26 | 0.0728 (15) | 0.0758 (15) | 0.0626 (15) | 0.0071 (12) | 0.0048 (12) | 0.0001 (11) |
| C27 | 0.096 (2) | 0.134 (3) | 0.0759 (19) | 0.0109 (17) | 0.0303 (16) | 0.0143 (16) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Fe—C10 | 2.0250 (18) | C12—H12 | 0.893 (14) |
| Fe—C4 | 2.025 (2) | C13—C14 | 1.469 (2) |
| Fe—C6 | 2.0255 (17) | C14—C15 | 1.386 (3) |
| Fe—C1 | 2.026 (2) | C14—C19 | 1.391 (2) |
| Fe—C3 | 2.028 (2) | C15—C16 | 1.372 (3) |

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| Fe—C5 | 2.031 (2) | C15—H15 | 0.9300 |
| Fe—C2 | 2.032 (2) | C16—C17 | 1.384 (3) |
| Fe—C9 | 2.0336 (18) | C16—H16 | 0.9300 |
| Fe—C7 | 2.0421 (17) | C17—C18 | 1.383 (3) |
| Fe—C8 | 2.0442 (18) | C18—C19 | 1.368 (3) |
| O1—C11 | 1.285 (2) | C18—H18 | 0.9300 |
| O2—C13 | 1.295 (2) | C19—H19 | 0.9300 |
| O2—H2A | 0.852 (17) | C20—C21 | 1.497 (3) |
| O3—C17 | 1.359 (2) | C20—H20A | 0.9700 |
| O3—C20 | 1.432 (2) | C20—H20B | 0.9700 |
| C1—C2 | 1.406 (3) | C21—C22 | 1.513 (3) |
| C1—C5 | 1.421 (3) | C21—H21A | 0.9700 |
| C1—H1 | 0.9300 | C21—H21B | 0.9700 |
| C2—C3 | 1.382 (3) | C22—C23 | 1.519 (3) |
| C2—H2 | 0.9300 | C22—H22A | 0.9700 |
| C3—C4 | 1.389 (4) | C22—H22B | 0.9700 |
| C3—H3 | 0.9300 | C23—C24 | 1.507 (3) |
| C4—C5 | 1.390 (4) | C23—H23A | 0.9700 |
| C4—H4 | 0.9300 | C23—H23B | 0.9700 |
| C5—H5 | 0.9300 | C24—C25 | 1.512 (3) |
| C6—C7 | 1.411 (3) | C24—H24A | 0.9700 |
| C6—C10 | 1.423 (2) | C24—H24B | 0.9700 |
| C6—H6 | 0.9300 | C25—C26 | 1.509 (3) |
| C7—C8 | 1.408 (3) | C25—H25A | 0.9700 |
| C7—H7 | 0.9300 | C25—H25B | 0.9700 |
| C8—C9 | 1.409 (3) | C26—C27 | 1.507 (3) |
| C8—H8 | 0.9300 | C26—H26A | 0.9700 |
| C9—C10 | 1.432 (2) | C26—H26B | 0.9700 |
| C9—H9 | 0.9300 | C27—H27A | 0.9600 |
| C10—C11 | 1.462 (2) | C27—H27B | 0.9600 |
| C11—C12 | 1.398 (3) | C27—H27C | 0.9600 |
| C12—C13 | 1.387 (2) | | |
| C10—Fe—C4 | 161.12 (10) | C9—C8—Fe | 69.38 (10) |
| C10—Fe—C6 | 41.12 (7) | C7—C8—H8 | 125.7 |
| C4—Fe—C6 | 156.54 (11) | C9—C8—H8 | 125.7 |
| C10—Fe—C1 | 108.46 (8) | Fe—C8—H8 | 126.7 |
| C4—Fe—C1 | 67.75 (10) | C8—C9—C10 | 107.91 (17) |
| C6—Fe—C1 | 124.02 (9) | C8—C9—Fe | 70.19 (11) |
| C10—Fe—C3 | 157.43 (10) | C10—C9—Fe | 69.02 (10) |
| C4—Fe—C3 | 40.09 (11) | C8—C9—H9 | 126.0 |
| C6—Fe—C3 | 121.15 (10) | C10—C9—H9 | 126.0 |
| C1—Fe—C3 | 67.61 (10) | Fe—C9—H9 | 126.3 |
| C10—Fe—C5 | 124.92 (10) | C6—C10—C9 | 107.01 (16) |
| C4—Fe—C5 | 40.07 (10) | C6—C10—C11 | 126.99 (16) |
| C6—Fe—C5 | 161.49 (9) | C9—C10—C11 | 125.87 (17) |
| C1—Fe—C5 | 41.02 (9) | C6—C10—Fe | 69.46 (10) |
| C3—Fe—C5 | 67.75 (11) | C9—C10—Fe | 69.66 (10) |
| C10—Fe—C2 | 122.71 (9) | C11—C10—Fe | 122.85 (12) |
| C4—Fe—C2 | 67.33 (10) | O1—C11—C12 | 120.75 (17) |

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| C6—Fe—C2 | 107.27 (9) | O1—C11—C10 | 118.08 (16) |
| C1—Fe—C2 | 40.54 (10) | C12—C11—C10 | 121.16 (16) |
| C3—Fe—C2 | 39.79 (9) | C13—C12—C11 | 121.90 (17) |
| C5—Fe—C2 | 68.30 (9) | C13—C12—H12 | 120.6 (12) |
| C10—Fe—C9 | 41.33 (7) | C11—C12—H12 | 117.5 (12) |
| C4—Fe—C9 | 124.16 (10) | O2—C13—C12 | 120.18 (16) |
| C6—Fe—C9 | 68.86 (7) | O2—C13—C14 | 116.77 (16) |
| C1—Fe—C9 | 123.98 (10) | C12—C13—C14 | 123.05 (16) |
| C3—Fe—C9 | 159.41 (10) | C15—C14—C19 | 117.14 (17) |
| C5—Fe—C9 | 108.68 (9) | C15—C14—C13 | 122.06 (16) |
| C2—Fe—C9 | 159.72 (9) | C19—C14—C13 | 120.80 (17) |
| C10—Fe—C7 | 68.81 (8) | C16—C15—C14 | 122.14 (17) |
| C4—Fe—C7 | 121.45 (10) | C16—C15—H15 | 118.9 |
| C6—Fe—C7 | 40.59 (8) | C14—C15—H15 | 118.9 |
| C1—Fe—C7 | 159.49 (10) | C15—C16—C17 | 119.78 (19) |
| C3—Fe—C7 | 106.66 (10) | C15—C16—H16 | 120.1 |
| C5—Fe—C7 | 157.09 (10) | C17—C16—H16 | 120.1 |
| C2—Fe—C7 | 122.56 (9) | O3—C17—C18 | 116.99 (17) |
| C9—Fe—C7 | 68.28 (8) | O3—C17—C16 | 124.08 (18) |
| C10—Fe—C8 | 68.74 (7) | C18—C17—C16 | 118.92 (18) |
| C4—Fe—C8 | 107.89 (9) | C19—C18—C17 | 120.75 (18) |
| C6—Fe—C8 | 68.21 (8) | C19—C18—H18 | 119.6 |
| C1—Fe—C8 | 159.36 (10) | C17—C18—H18 | 119.6 |
| C3—Fe—C8 | 122.98 (9) | C18—C19—C14 | 121.25 (19) |
| C5—Fe—C8 | 122.63 (9) | C18—C19—H19 | 119.4 |
| C2—Fe—C8 | 158.36 (10) | C14—C19—H19 | 119.4 |
| C9—Fe—C8 | 40.43 (7) | O3—C20—C21 | 108.64 (16) |
| C7—Fe—C8 | 40.31 (8) | O3—C20—H20A | 110.0 |
| C13—O2—H2A | 108 (2) | C21—C20—H20A | 110.0 |
| C17—O3—C20 | 118.13 (15) | O3—C20—H20B | 110.0 |
| C2—C1—C5 | 107.6 (2) | C21—C20—H20B | 110.0 |
| C2—C1—Fe | 69.98 (12) | H20A—C20—H20B | 108.3 |
| C5—C1—Fe | 69.70 (12) | C20—C21—C22 | 112.67 (17) |
| C2—C1—H1 | 126.2 | C20—C21—H21A | 109.1 |
| C5—C1—H1 | 126.2 | C22—C21—H21A | 109.1 |
| Fe—C1—H1 | 125.7 | C20—C21—H21B | 109.1 |
| C3—C2—C1 | 108.0 (2) | C22—C21—H21B | 109.1 |
| C3—C2—Fe | 69.94 (12) | H21A—C21—H21B | 107.8 |
| C1—C2—Fe | 69.48 (12) | C21—C22—C23 | 113.50 (17) |
| C3—C2—H2 | 126.0 | C21—C22—H22A | 108.9 |
| C1—C2—H2 | 126.0 | C23—C22—H22A | 108.9 |
| Fe—C2—H2 | 126.2 | C21—C22—H22B | 108.9 |
| C2—C3—C4 | 108.5 (2) | C23—C22—H22B | 108.9 |
| C2—C3—Fe | 70.27 (13) | H22A—C22—H22B | 107.7 |
| C4—C3—Fe | 69.85 (14) | C24—C23—C22 | 114.03 (17) |
| C2—C3—H3 | 125.7 | C24—C23—H23A | 108.7 |
| C4—C3—H3 | 125.7 | C22—C23—H23A | 108.7 |
| Fe—C3—H3 | 125.7 | C24—C23—H23B | 108.7 |
| C3—C4—C5 | 109.0 (2) | C22—C23—H23B | 108.7 |

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| C3—C4—Fe | 70.06 (13) | H23A—C23—H23B | 107.6 |
| C5—C4—Fe | 70.20 (12) | C23—C24—C25 | 114.73 (18) |
| C3—C4—H4 | 125.5 | C23—C24—H24A | 108.6 |
| C5—C4—H4 | 125.5 | C25—C24—H24A | 108.6 |
| Fe—C4—H4 | 125.8 | C23—C24—H24B | 108.6 |
| C4—C5—C1 | 106.9 (2) | C25—C24—H24B | 108.6 |
| C4—C5—Fe | 69.74 (13) | H24A—C24—H24B | 107.6 |
| C1—C5—Fe | 69.28 (12) | C26—C25—C24 | 113.94 (19) |
| C4—C5—H5 | 126.6 | C26—C25—H25A | 108.8 |
| C1—C5—H5 | 126.6 | C24—C25—H25A | 108.8 |
| Fe—C5—H5 | 126.0 | C26—C25—H25B | 108.8 |
| C7—C6—C10 | 108.40 (16) | C24—C25—H25B | 108.8 |
| C7—C6—Fe | 70.34 (10) | H25A—C25—H25B | 107.7 |
| C10—C6—Fe | 69.42 (10) | C27—C26—C25 | 113.5 (2) |
| C7—C6—H6 | 125.8 | C27—C26—H26A | 108.9 |
| C10—C6—H6 | 125.8 | C25—C26—H26A | 108.9 |
| Fe—C6—H6 | 126.0 | C27—C26—H26B | 108.9 |
| C8—C7—C6 | 108.10 (17) | C25—C26—H26B | 108.9 |
| C8—C7—Fe | 69.93 (10) | H26A—C26—H26B | 107.7 |
| C6—C7—Fe | 69.07 (10) | C26—C27—H27A | 109.5 |
| C8—C7—H7 | 126.0 | C26—C27—H27B | 109.5 |
| C6—C7—H7 | 126.0 | H27A—C27—H27B | 109.5 |
| Fe—C7—H7 | 126.6 | C26—C27—H27C | 109.5 |
| C7—C8—C9 | 108.58 (17) | H27A—C27—H27C | 109.5 |
| C7—C8—Fe | 69.77 (10) | H27B—C27—H27C | 109.5 |
| C10—Fe—C1—C2 | −119.09 (14) | C3—Fe—C7—C8 | 121.69 (14) |
| C4—Fe—C1—C2 | 80.65 (16) | C5—Fe—C7—C8 | 49.6 (3) |
| C6—Fe—C1—C2 | −76.22 (16) | C2—Fe—C7—C8 | 162.18 (12) |
| C3—Fe—C1—C2 | 37.16 (15) | C9—Fe—C7—C8 | −37.15 (11) |
| C5—Fe—C1—C2 | 118.5 (2) | C10—Fe—C7—C6 | 37.88 (11) |
| C9—Fe—C1—C2 | −162.22 (12) | C4—Fe—C7—C6 | −159.86 (13) |
| C7—Fe—C1—C2 | −40.4 (3) | C1—Fe—C7—C6 | −48.3 (3) |
| C8—Fe—C1—C2 | 162.3 (2) | C3—Fe—C7—C6 | −118.71 (13) |
| C10—Fe—C1—C5 | 122.40 (15) | C5—Fe—C7—C6 | 169.2 (2) |
| C4—Fe—C1—C5 | −37.86 (15) | C2—Fe—C7—C6 | −78.23 (15) |
| C6—Fe—C1—C5 | 165.27 (14) | C9—Fe—C7—C6 | 82.44 (12) |
| C3—Fe—C1—C5 | −81.35 (17) | C8—Fe—C7—C6 | 119.59 (17) |
| C2—Fe—C1—C5 | −118.5 (2) | C6—C7—C8—C9 | 0.0 (2) |
| C9—Fe—C1—C5 | 79.26 (16) | Fe—C7—C8—C9 | 58.68 (13) |
| C7—Fe—C1—C5 | −158.9 (2) | C6—C7—C8—Fe | −58.70 (13) |
| C8—Fe—C1—C5 | 43.8 (3) | C10—Fe—C8—C7 | 81.90 (12) |
| C5—C1—C2—C3 | 0.3 (2) | C4—Fe—C8—C7 | −117.83 (15) |
| Fe—C1—C2—C3 | −59.55 (15) | C6—Fe—C8—C7 | 37.54 (11) |
| C5—C1—C2—Fe | 59.82 (14) | C1—Fe—C8—C7 | 167.9 (2) |
| C10—Fe—C2—C3 | −160.68 (15) | C3—Fe—C8—C7 | −76.33 (16) |
| C4—Fe—C2—C3 | 37.44 (16) | C5—Fe—C8—C7 | −159.40 (14) |
| C6—Fe—C2—C3 | −118.23 (16) | C2—Fe—C8—C7 | −44.4 (3) |
| C1—Fe—C2—C3 | 119.2 (2) | C9—Fe—C8—C7 | 120.10 (16) |
| C5—Fe—C2—C3 | 80.85 (17) | C10—Fe—C8—C9 | −38.20 (11) |

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| C9—Fe—C2—C3 | 166.1 (2) | C4—Fe—C8—C9 | 122.07 (14) |
| C7—Fe—C2—C3 | −76.40 (18) | C6—Fe—C8—C9 | −82.56 (12) |
| C8—Fe—C2—C3 | −43.9 (3) | C1—Fe—C8—C9 | 47.8 (3) |
| C10—Fe—C2—C1 | 80.10 (15) | C3—Fe—C8—C9 | 163.58 (14) |
| C4—Fe—C2—C1 | −81.78 (16) | C5—Fe—C8—C9 | 80.50 (15) |
| C6—Fe—C2—C1 | 122.55 (13) | C2—Fe—C8—C9 | −164.5 (2) |
| C3—Fe—C2—C1 | −119.2 (2) | C7—Fe—C8—C9 | −120.10 (16) |
| C5—Fe—C2—C1 | −38.37 (14) | C7—C8—C9—C10 | 0.0 (2) |
| C9—Fe—C2—C1 | 46.9 (3) | Fe—C8—C9—C10 | 58.91 (12) |
| C7—Fe—C2—C1 | 164.38 (13) | C7—C8—C9—Fe | −58.91 (13) |
| C8—Fe—C2—C1 | −163.2 (2) | C10—Fe—C9—C8 | 119.22 (16) |
| C1—C2—C3—C4 | −0.3 (3) | C4—Fe—C9—C8 | −77.06 (15) |
| Fe—C2—C3—C4 | −59.59 (16) | C6—Fe—C9—C8 | 80.79 (12) |
| C1—C2—C3—Fe | 59.26 (15) | C1—Fe—C9—C8 | −161.63 (12) |
| C10—Fe—C3—C2 | 46.5 (3) | C3—Fe—C9—C8 | −42.4 (3) |
| C4—Fe—C3—C2 | −119.4 (2) | C5—Fe—C9—C8 | −118.74 (13) |
| C6—Fe—C3—C2 | 79.42 (17) | C2—Fe—C9—C8 | 163.4 (2) |
| C1—Fe—C3—C2 | −37.85 (14) | C7—Fe—C9—C8 | 37.05 (11) |
| C5—Fe—C3—C2 | −82.36 (16) | C4—Fe—C9—C10 | 163.72 (13) |
| C9—Fe—C3—C2 | −166.3 (2) | C6—Fe—C9—C10 | −38.43 (10) |
| C7—Fe—C3—C2 | 121.23 (15) | C1—Fe—C9—C10 | 79.14 (14) |
| C8—Fe—C3—C2 | 162.24 (14) | C3—Fe—C9—C10 | −161.6 (3) |
| C10—Fe—C3—C4 | 165.9 (2) | C5—Fe—C9—C10 | 122.04 (12) |
| C6—Fe—C3—C4 | −161.16 (14) | C2—Fe—C9—C10 | 44.2 (3) |
| C1—Fe—C3—C4 | 81.57 (17) | C7—Fe—C9—C10 | −82.18 (12) |
| C5—Fe—C3—C4 | 37.06 (15) | C8—Fe—C9—C10 | −119.22 (16) |
| C2—Fe—C3—C4 | 119.4 (2) | C7—C6—C10—C9 | −0.1 (2) |
| C9—Fe—C3—C4 | −46.9 (3) | Fe—C6—C10—C9 | −59.81 (12) |
| C7—Fe—C3—C4 | −119.35 (16) | C7—C6—C10—C11 | 176.05 (17) |
| C8—Fe—C3—C4 | −78.34 (18) | Fe—C6—C10—C11 | 116.30 (18) |
| C2—C3—C4—C5 | 0.3 (3) | C7—C6—C10—Fe | 59.76 (13) |
| Fe—C3—C4—C5 | −59.59 (15) | C8—C9—C10—C6 | 0.0 (2) |
| C2—C3—C4—Fe | 59.85 (16) | Fe—C9—C10—C6 | 59.68 (12) |
| C10—Fe—C4—C3 | −163.2 (2) | C8—C9—C10—C11 | −176.12 (16) |
| C6—Fe—C4—C3 | 44.0 (3) | Fe—C9—C10—C11 | −116.48 (18) |
| C1—Fe—C4—C3 | −81.20 (17) | C8—C9—C10—Fe | −59.64 (12) |
| C5—Fe—C4—C3 | −119.9 (2) | C4—Fe—C10—C6 | −164.0 (3) |
| C2—Fe—C4—C3 | −37.16 (15) | C1—Fe—C10—C6 | 120.97 (13) |
| C9—Fe—C4—C3 | 161.92 (14) | C3—Fe—C10—C6 | 45.1 (3) |
| C7—Fe—C4—C3 | 78.19 (17) | C5—Fe—C10—C6 | 163.49 (12) |
| C8—Fe—C4—C3 | 120.30 (15) | C2—Fe—C10—C6 | 78.52 (14) |
| C10—Fe—C4—C5 | −43.2 (3) | C9—Fe—C10—C6 | −118.18 (15) |
| C6—Fe—C4—C5 | 163.89 (18) | C7—Fe—C10—C6 | −37.40 (11) |
| C1—Fe—C4—C5 | 38.74 (15) | C8—Fe—C10—C6 | −80.78 (12) |
| C3—Fe—C4—C5 | 119.9 (2) | C4—Fe—C10—C9 | −45.8 (3) |
| C2—Fe—C4—C5 | 82.77 (16) | C6—Fe—C10—C9 | 118.18 (15) |
| C9—Fe—C4—C5 | −78.14 (17) | C1—Fe—C10—C9 | −120.85 (13) |
| C7—Fe—C4—C5 | −161.87 (13) | C3—Fe—C10—C9 | 163.2 (2) |
| C8—Fe—C4—C5 | −119.76 (15) | C5—Fe—C10—C9 | −78.33 (13) |

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| C3—C4—C5—C1 | −0.1 (3) | C2—Fe—C10—C9 | −163.30 (12) |
| Fe—C4—C5—C1 | −59.60 (14) | C7—Fe—C10—C9 | 80.78 (12) |
| C3—C4—C5—Fe | 59.51 (16) | C8—Fe—C10—C9 | 37.39 (11) |
| C2—C1—C5—C4 | −0.1 (2) | C4—Fe—C10—C11 | 74.5 (3) |
| Fe—C1—C5—C4 | 59.89 (15) | C6—Fe—C10—C11 | −121.53 (19) |
| C2—C1—C5—Fe | −60.00 (14) | C1—Fe—C10—C11 | −0.56 (18) |
| C10—Fe—C5—C4 | 164.31 (14) | C3—Fe—C10—C11 | −76.5 (3) |
| C6—Fe—C5—C4 | −159.6 (2) | C5—Fe—C10—C11 | 41.96 (19) |
| C1—Fe—C5—C4 | −118.1 (2) | C2—Fe—C10—C11 | −43.01 (18) |
| C3—Fe—C5—C4 | −37.08 (15) | C9—Fe—C10—C11 | 120.29 (19) |
| C2—Fe—C5—C4 | −80.13 (17) | C7—Fe—C10—C11 | −158.93 (17) |
| C9—Fe—C5—C4 | 121.26 (15) | C8—Fe—C10—C11 | 157.69 (17) |
| C7—Fe—C5—C4 | 43.0 (3) | C6—C10—C11—O1 | −178.33 (17) |
| C8—Fe—C5—C4 | 78.79 (18) | C9—C10—C11—O1 | −2.9 (3) |
| C10—Fe—C5—C1 | −77.63 (17) | Fe—C10—C11—O1 | −90.42 (19) |
| C4—Fe—C5—C1 | 118.1 (2) | C6—C10—C11—C12 | 2.8 (3) |
| C6—Fe—C5—C1 | −41.6 (3) | C9—C10—C11—C12 | 178.15 (17) |
| C3—Fe—C5—C1 | 80.98 (17) | Fe—C10—C11—C12 | 90.66 (19) |
| C2—Fe—C5—C1 | 37.93 (15) | O1—C11—C12—C13 | −2.0 (3) |
| C9—Fe—C5—C1 | −120.68 (15) | C10—C11—C12—C13 | 176.85 (17) |
| C7—Fe—C5—C1 | 161.1 (2) | C11—C12—C13—O2 | 1.1 (3) |
| C8—Fe—C5—C1 | −163.15 (14) | C11—C12—C13—C14 | −178.12 (17) |
| C10—Fe—C6—C7 | −119.49 (16) | O2—C13—C14—C15 | 172.73 (18) |
| C4—Fe—C6—C7 | 47.5 (3) | C12—C13—C14—C15 | −8.0 (3) |
| C1—Fe—C6—C7 | 161.61 (14) | O2—C13—C14—C19 | −6.7 (3) |
| C3—Fe—C6—C7 | 79.02 (15) | C12—C13—C14—C19 | 172.56 (18) |
| C5—Fe—C6—C7 | −166.7 (2) | C19—C14—C15—C16 | 1.1 (3) |
| C2—Fe—C6—C7 | 120.23 (13) | C13—C14—C15—C16 | −178.35 (19) |
| C9—Fe—C6—C7 | −80.87 (13) | C14—C15—C16—C17 | −0.8 (3) |
| C8—Fe—C6—C7 | −37.29 (12) | C20—O3—C17—C18 | 178.74 (19) |
| C4—Fe—C6—C10 | 167.0 (2) | C20—O3—C17—C16 | −0.5 (3) |
| C1—Fe—C6—C10 | −78.90 (15) | C15—C16—C17—O3 | 178.73 (19) |
| C3—Fe—C6—C10 | −161.49 (12) | C15—C16—C17—C18 | −0.5 (3) |
| C5—Fe—C6—C10 | −47.2 (3) | O3—C17—C18—C19 | −177.85 (19) |
| C2—Fe—C6—C10 | −120.28 (12) | C16—C17—C18—C19 | 1.5 (3) |
| C9—Fe—C6—C10 | 38.61 (10) | C17—C18—C19—C14 | −1.1 (3) |
| C7—Fe—C6—C10 | 119.49 (16) | C15—C14—C19—C18 | −0.2 (3) |
| C8—Fe—C6—C10 | 82.20 (12) | C13—C14—C19—C18 | 179.31 (18) |
| C10—C6—C7—C8 | 0.0 (2) | C17—O3—C20—C21 | −178.62 (17) |
| Fe—C6—C7—C8 | 59.23 (13) | O3—C20—C21—C22 | −179.53 (17) |
| C10—C6—C7—Fe | −59.18 (12) | C20—C21—C22—C23 | 178.09 (18) |
| C10—Fe—C7—C8 | −81.71 (12) | C21—C22—C23—C24 | 177.94 (18) |
| C4—Fe—C7—C8 | 80.55 (16) | C22—C23—C24—C25 | 180.00 (18) |
| C6—Fe—C7—C8 | −119.59 (17) | C23—C24—C25—C26 | 177.61 (18) |
| C1—Fe—C7—C8 | −167.9 (2) | C24—C25—C26—C27 | 178.1 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| O2—H2A···O1 | 0.852 (17) | 1.72 (2) | 2.499 (2) | 151 (3) |

**Fig. 1**

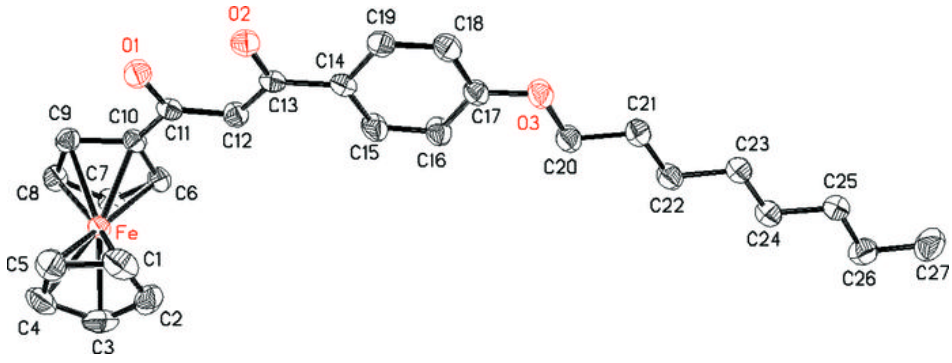

**Fig. 2**

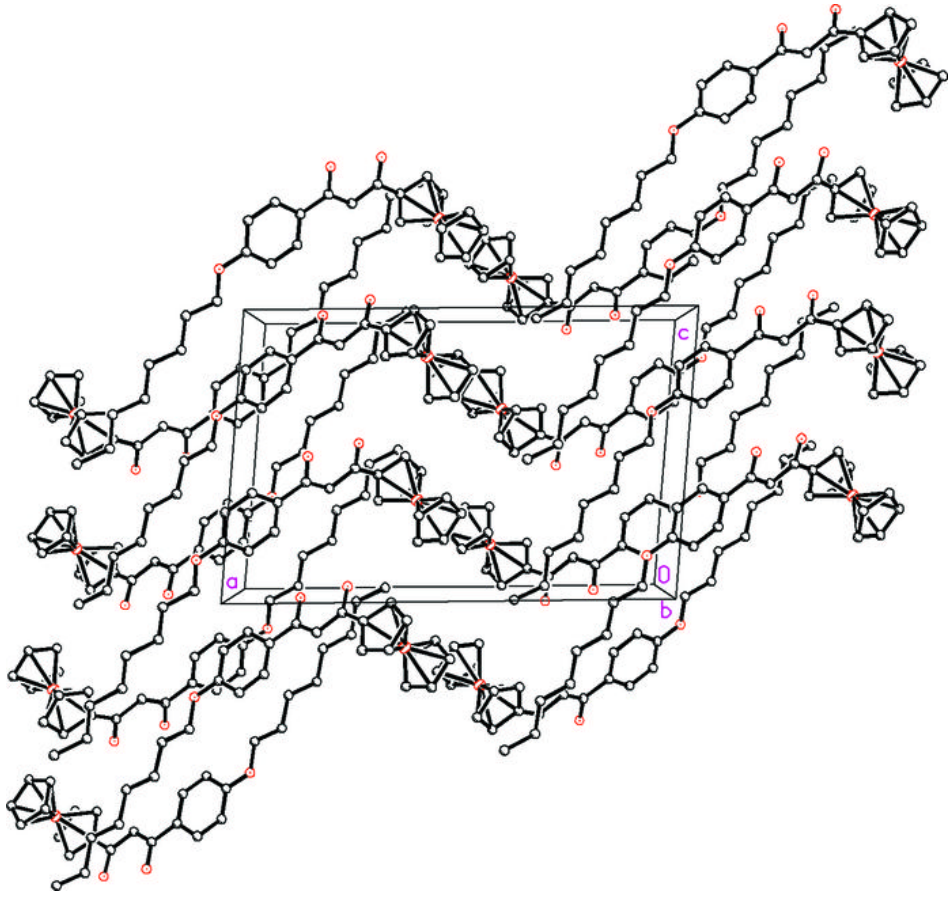

**Fig. 3**