The structure was determined by direct methods and refined by anistropic full-matrix least squares on *F*. All C atoms were refined isotropically. All H atoms were located geometrically (C—H distance 0.98 Å) and not refined.

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Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55836 (22 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SH1022]

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Structures of 1-Ferrocenyl-1-phenylethanol, Ferrocenyl(diphenyl)methanol and Ferrocene-1,1′-diylbis(diphenylmethanol)

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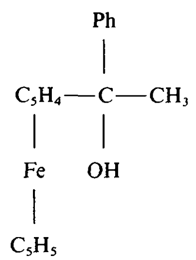
Abstract

Racemic 1-ferrocenyl-1-phenylethanol, $[(C_5H_5)Fe(C_5H_4)]CPhMeOH$ (I), crystallizes as discrete molecules which are not involved in hydrogen bonding; the shortest intermolecular O···O contact is 3.768(3) Å and the hydroxyl H atom is orientated towards the unsubstituted cyclopentadienyl ring. Ferrocenyl(diphenyl)methanol, $[(C_5H_5)Fe(C_5H_4)]CPh_2OH$ (II) is hydrogen bonded to form centrosymmetric dimers with O···O 2.816(1) and H···O 2.52 Å. Ferrocene-1,1′-diylbis(diphenylmethanol), $Fe[(C_5H_4)C(Ph)_2COH]_2$ (III) crystallizes as a dimeric aggregate with the Fe atoms on twofold crystallographic symmetry axes and the four O atoms defining a folded trapezium with O···O 2.762(2), 2.714(2) and 2.865(2) Å. The four hydroxyl groups are disordered equally over two orientations such that there are two half-occupancy H-atom sites between each hydrogen-bonded oxygen pair.

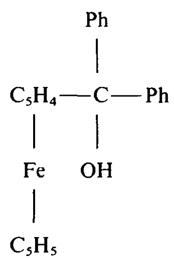
Comment

Triphenylmethanol, Ph_3COH, crystallizes as hydrogen-bonded tetrameric aggregates with threefold crystallographic symmetry, each containing an approximately tetrahedral arrangement of O atoms with necessarily disordered hydroxyl H atoms (Ferguson, Gallagher, Glidewell, Low & Scrimgeour, 1992). These aggregates are significantly different from the cyclic tetrameric aggregates found in triphenylsilanol, Ph_3SiOH (Puff, Braun & Reuter, 1991), and in triphenylgermanol, Ph_3GeOH (Ferguson, Gallagher, Murphy, Spalding, Glidewell & Holden, 1992), whose graph set (Etter, MacDonald & Bernstein, 1990) is $R_4^4(8)$. Triphenylmethanol can act as a host towards guest molecules such as methanol and dimethyl sulfoxide (Weber, Skobridis & Goldberg, 1989) albeit with hydrogen-bonding arrangements wholly different from that in unsolvated Ph_3COH. The diol *m*-bis(diphenylhydroxymethyl)benzene, which forms similar host/guest aggregates with a range of different guest species, crystallizes as centrosymmetric dimers (Toda, Kai, Toyotaka, Yip & Mak, 1989) with graph set $R_2^2(16)$.

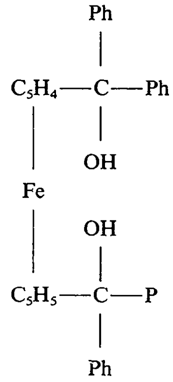
In order to assess the effect on the hydrogen-bonding patterns in the crystal lattice in alcohols of this general type by altering the steric demands at the central C atom, we have now determined the structures of racemic 1-ferrocenyl-1-phenylethanol, $[(C_5H_5)Fe(C_5H_4)]CPhMeOH$ (I); ferrocenyl(diphenyl)methanol, $[(C_5H_5)Fe(C_5H_4)]CPh_2OH$ (II); and ferrocene-1,1′-diylbis(diphenylmethanol), $Fe[(C_5H_4)C(Ph)_2COH]_2$ (III).



(I)



(II)



(III)

$[(C_5H_5)Fe(C_5H_4)]CPhMeOH$ (I) (Fig. 1) crystallizes in the centrosymetric space group $P2_1/n$ with one molecule in the asymmetric unit; consequently *R* and *S* enantiomers are present in equal numbers and related by crystallographic centres of inversion. The unsubstituted C_5H_5 ring is disordered over two sites with occupancies of 87 and 13% for the major and minor components. There is no hydrogen bonding in the crystal structure, presumably because the conformation adopted by the ferrocenyl, methyl and phenyl substitutents in the solid state shields the hydroxyl group; the distance between the nearest hydroxyl O atoms O···O, 3.768(3) Å, precludes O—H···O hydrogen bonding. Instead the hydroxyl H atom (which was clearly located in difference maps) is orientated towards the C_5H_5 cyclopentadienyl ring with dimensions O—H 0.76 Å and C—O—H 105°.

Ferrocenyl(diphenyl)methanol (II) (Fig. 2) differs from the triphenylmethanol molecule by replacement of one of the phenyl groups by a ferrocenyl group. As in 1-ferrocenyl-1-phenylethanol (I) the hydroxyl H atom, the position of which was clearly located from a difference map, is directed towards the unsubstituted C_5H_5 ring in the same molecule (Fig. 2). An unexpected feature in (II) is that the shortest O···O contact between adjacent molecules related by an inversion centre is 2.816(1) Å with O—H 0.76, H···O 2.52 Å, C—O—H 104, O—H···O 106°. The graph set for this centrosymmetric hydrogen-bonded motif is $R_2^2(4)$. It is of interest that the closest intermolecular approach in (I) [3.768(3) Å] is appreciably longer than in (II) [2.816(2) Å] although the steric congestion about the unique central C atom in (II) is apparently greater than in (I).

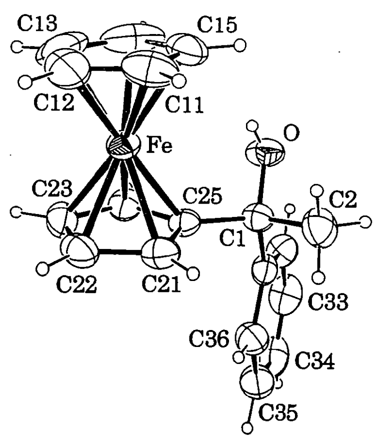


Fig. 1. A view of 1-ferrocenyl-1-phenylethanol (I). The non-H atoms are shown with thermal ellipsoids drawn at the 50% probability level. For clarity the minor cyclopentadienyl site has been omitted and the H atoms are drawn as small spheres of an arbitrary size.

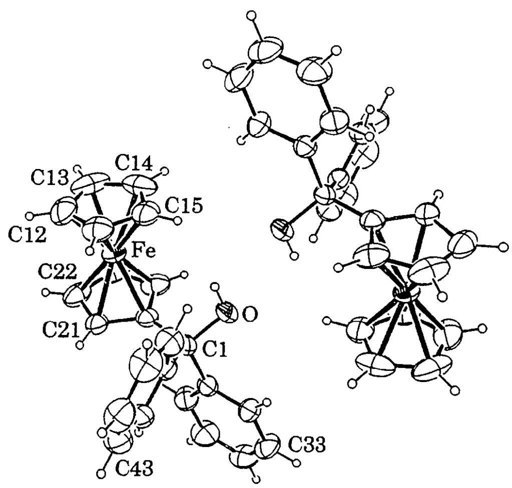


Fig. 2. A view of ferrocenyl(diphenyl)methanol (II) as the dimeric aggregate. Ellipsoid conditions are as for Fig. 1.

Ferrocene-1,1′-diylbis(diphenylmethanol) (III) differs from (I) and (II) in that it contains two carbinol moieties on the electroactive molecular core. The asymmetric unit in this structure comprises two independent half-molecules with both Fe atoms lying on a crystallographic twofold axis. The molecules are hydrogen bonded to form a dimeric structural motif, graph set $R_4^4(8)$ (Fig. 3) which is quite different from that found in triphenylmethanol. The O atoms form a flattened trapezium with O···O hydrogen-bond distances 2.762(2) (×2), 2.714(2) and 2.865(2) Å. Difference-density maps showed that in both molecules the hydroxyl H atom is disordered equally over two sites, each directed towards neighbouring hydroxyl O atoms as shown in Fig. 3. The O—H distances are in the range 0.60 to 0.70 Å while the C—O—H angles are between 116.3 and 125.7°. The positional disorder of the H atoms demands that the hydrogen-bonded motif describes either a clockwise or a counterclockwise pattern; hence each individual dimeric aggregate must be chiral, with equal numbers of the two enantiomers rendering the crystal as a whole achiral.

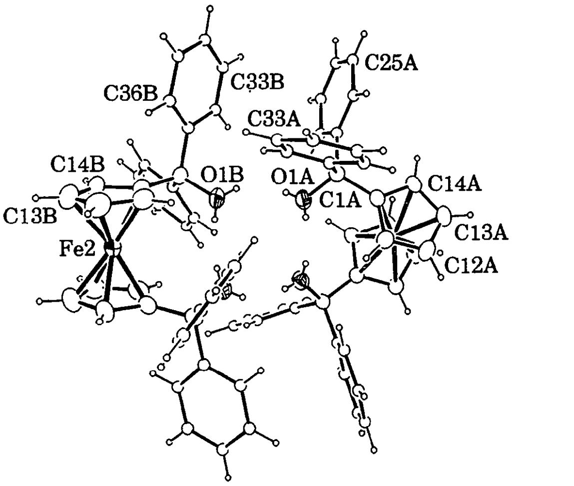


Fig. 3. A view of the two independent ferrocene-1,1′-diylbis(diphenylmethanol) molecules (III). The non-H atoms are depicted with thermal ellipsoids drawn at the 35% probability level. For clarity the H atoms are drawn as small spheres of an arbitrary size. A crystallographic twofold axis passes through the two Fe atoms.

In (I) the major conformer has a 3.4(3)° angle between the C_5 planes of the ferrocene moiety which is within 8.8(3)° of an eclipsed conformation [the relevant values for the minor isomer are 7(1) and 25(1)°, respectively]; in (II) the corresponding dihedral angle is 3.2(1)° and the rotation of the C_5 planes out of an eclipsed conformation is 17.6(1)°. The two independent ferrocene moieties in (III) have 3.7(2) and 4.6(2)° dihedral angles between their symmetry related C_5 planes (for molecules *A* and *B*, respectively). Although the C_5 rings are within 3.2(2) and 7.7(2)° of being eclipsed, the conformation adopted is such that the exocyclic C atoms are rotated about a line joining the ring centroids through −66.5(2) and 62.1(2)° from an eclipsed conformation.

The molecular dimensions for (I), (II) and (III) are summarized in Table 4 and show no unusual features. There is no solvent of crystallization present in any of the lattices and an examination of the structures using *PLATON* (Spek, 1991) reveals no potential volume for any solvent molecules.

Experimental

Compound (I)

Crystal data

$C_{18}H_{18}FeO$
M_r = 305.53
Monoclinic
$P2_1/n$
a = 13.7594 (6) Å
b = 5.9786 (3) Å
c = 17.8430 (12) Å
β = 106.115 (5)°
V = 1410.12 (13) Å^3
Z = 4

D_x = 1.439 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.70930 Å
Cell parameters from 25 reflections
θ = 10.5–15.8°
μ = 1.06 mm^{-1}
T = 293 K
Block
0.30 × 0.25 × 0.20 mm
Red-brown

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical
T_{min} = 0.6940, T_{max} = 0.7878
5831 measured reflections
3069 independent reflections
2293 observed reflections [$I_{net} > 3.0\sigma(I_{net})$]

R_{int} = 0.012
θ_{max} = 26.91°
h = −17 → 16
k = 0 → 7
l = 0 → 22
3 standard reflections
frequency: 120 min
intensity variation: −2.0%

Refinement

Refinement on F
Final R = 0.025
wR = 0.034
S = 1.25
2293 reflections
197 parameters
O—H from Δ maps; C—H, 0.95 Å riding
$w = 1/[\sigma^2(F)+0.0004F^2]$
$(\Delta/\sigma)_{max}$ = 0.023

$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 10162 (3776)
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *for* (I)

$$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Fe	0.286552 (22)	0.20604 (5)	0.076972 (16)	0.03530 (17)
O	0.09022 (13)	−0.0505 (3)	−0.06064 (10)	0.0486 (10)
C1	0.11628 (15)	0.1617 (3)	−0.08809 (12)	0.0349 (10)
C2	0.03753 (18)	0.3333 (4)	−0.08193 (14)	0.0488 (14)
C11	0.2308 (6)	0.3070 (7)	0.1668 (3)	0.060 (3)
C12	0.3343 (5)	0.2647 (15)	0.19439 (21)	0.083 (4)
C13	0.3490 (5)	0.0433 (18)	0.1788 (3)	0.091 (4)
C14	0.2557 (7)	−0.0535 (6)	0.1408 (3)	0.073 (3)
C15	0.18242 (23)	0.1115 (12)	0.13396 (18)	0.0522 (19)
C21	0.25511 (17)	0.4417 (4)	−0.00932 (12)	0.0405 (12)
C22	0.36090 (18)	0.4307 (4)	0.02694 (12)	0.0479 (13)
C23	0.39360 (17)	0.2121 (5)	0.01785 (13)	0.0483 (13)
C24	0.30801 (17)	0.0860 (4)	−0.02451 (12)	0.0411 (12)
C25	0.22180 (15)	0.2281 (4)	−0.04103 (11)	0.0328 (10)
C31	0.11470 (15)	0.1291 (4)	−0.17322 (11)	0.0350 (10)
C32	0.07987 (18)	−0.0649 (4)	−0.21391 (13)	0.0467 (13)
C33	0.08037 (20)	−0.0855 (5)	−0.29133 (15)	0.0582 (15)
C34	0.11442 (19)	0.0833 (6)	−0.32861 (13)	0.0583 (17)
C35	0.14936 (19)	0.2772 (5)	−0.28892 (14)	0.0548 (15)
C36	0.14887 (17)	0.3004 (4)	−0.21195 (13)	0.0451 (12)
C11*A*	0.2998 (23)	0.3065 (22)	0.1852 (11)	0.023 (4)
C12*A*	0.3697 (10)	0.135 (3)	0.1864 (12)	0.041 (6)
C13*A*	0.3253 (20)	−0.0614 (23)	0.1553 (13)	0.049 (7)
C14*A*	0.2102 (15)	−0.003 (5)	0.1312 (12)	0.046 (7)
C15*A*	0.2009 (15)	0.224 (5)	0.1513 (13)	0.033 (5)
HO1	0.105	−0.040	−0.017	0.0620

Compound (II)

Crystal data

$C_{23}H_{20}FeO$
M_r = 368.25

D_x = 1.372 Mg m^{-3}
Mo $K\alpha$ radiation

Triclinic
$P\overline{1}$
a = 7.8205 (4) Å
b = 11.0274 (4) Å
c = 11.7715 (6) Å
α = 105.707 (4)°
β = 106.128 (5)°
γ = 102.403 (4)°
V = 891.45 (7) Å^3
Z = 2

λ = 0.70930 Å
Cell parameters from 25 reflections
θ = 9.50–25.50°
μ = 0.85 mm^{-1}
T = 293 K
Block
0.45 × 0.35 × 0.30 mm
Orange

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical
T_{min} = 0.7666, T_{max} = 0.8246
5174 measured reflections
5174 independent reflections

4294 observed reflections [I_{net}>3.0σ(I_{net})]
θ_{max} = 29.92°
h = −10 → 10
k = 0 → 15
l = −16 → 15
3 standard reflections
frequency: 60 min
intensity variation: none

Refinement

Refinement on F
Final R = 0.030
wR = 0.049
S = 1.46
4294 reflections
227 parameters
O—H from Δ maps; C—H, 0.95 Å riding
$w = 1/[\sigma^2(F)+0.0008F^2]$
$(\Delta/\sigma)_{max}$ <0.001

$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 9806 (914)
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 2. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *for* (II)

$$U_{eq} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Fe	0.80686 (3)	0.347480 (17)	0.224884 (19)	0.03852 (13)
O	0.67955 (15)	0.58033 (11)	0.08724 (10)	0.0506 (6)
C1	0.83751 (17)	0.63797 (12)	0.20420 (12)	0.0352 (6)
C11	0.58540 (25)	0.31522 (18)	0.28581 (18)	0.0562 (10)
C12	0.6864 (3)	0.22922 (22)	0.30722 (21)	0.0678 (13)
C13	0.6845 (3)	0.15185 (17)	0.1896 (3)	0.0764 (16)
C14	0.5807 (3)	0.19263 (19)	0.09583 (19)	0.0677 (11)
C15	0.51897 (22)	0.29383 (17)	0.15655 (18)	0.0535 (9)
C21	1.01030 (19)	0.52109 (14)	0.34689 (15)	0.0432 (7)
C22	1.08970 (23)	0.41550 (18)	0.32494 (22)	0.0600 (11)
C23	1.0546 (3)	0.36274 (17)	0.19415 (23)	0.0648 (13)
C24	0.9547 (3)	0.43523 (16)	0.13356 (17)	0.0528 (9)
C25	0.92675 (18)	0.53351 (13)	0.22774 (13)	0.0373 (7)
C31	0.97241 (19)	0.74859 (13)	0.18654 (12)	0.0370 (6)
C32	0.90303 (22)	0.84081 (15)	0.14459 (14)	0.0457 (8)
C33	1.0218 (3)	0.94478 (16)	0.13074 (17)	0.0573 (11)
C34	1.2089 (3)	0.95820 (17)	0.15892 (17)	0.0617 (11)
C35	1.2783 (3)	0.86868 (20)	0.20082 (19)	0.0612 (11)
C36	1.16077 (22)	0.76284 (17)	0.21437 (16)	0.0507 (9)
C41	0.77634 (18)	0.69752 (13)	0.31412 (12)	0.0362 (7)
C42	0.90471 (21)	0.80034 (15)	0.42249 (14)	0.0452 (8)
C43	0.8520 (3)	0.85157 (17)	0.52458 (16)	0.0568 (11)
C44	0.6727 (3)	0.79912 (20)	0.52030 (19)	0.0612 (12)
C45	0.54613 (25)	0.69710 (21)	0.41465 (20)	0.0608 (12)
C46	0.59592 (21)	0.64693 (17)	0.31113 (17)	0.0499 (9)
HO1	0.640	0.509	0.083	0.0528

Compound (III)

Crystal data

$C_{36}H_{30}FeO_2$
M_r = 550.47
Monoclinic
$C2/c$
a = 13.2841 (6) Å
b = 23.2856 (12) Å
c = 18.8106 (8) Å
β = 105.482 (4)°
V = 5607.5 (5) Å^3
Z = 8
D_x = 1.304 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.70930 Å
Cell parameters from 25 reflections
θ = 10.00–25.00°
μ = 0.57 mm^{-1}
T = 293 K
Block
0.75 × 0.60 × 0.60 mm
Orange

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical
T_{min} = 0.8333, T_{max} = 0.8774
6273 measured reflections
6095 independent reflections
4121 observed reflections [I_{net}>3.0σ(I_{net})]

R_{int} = 0.018
θ_{max} = 26.91°
h = −16 → 16
k = 0 → 29
l = 0 → 23
3 standard reflections
frequency: 120 min
intensity variation: −2.0%

Refinement

Refinement on F
Final R = 0.036
wR = 0.049
S = 1.37
4121 reflections
354 parameters
C—H, 0.95 Å riding; O—H from Δ maps
$w = 1/[\sigma^2(F)+0.0006F^2]$
$(\Delta/\sigma)_{max}$ = 0.007

$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Extinction correction: Larson (1970)
Extinction coefficient: 4275 (1274)
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 3. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *for* (III)

$$U_{eq} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Fe1	0.00000	0.365480 (18)	0.25000	0.0349 (3)
O1*A*	0.05084 (15)	0.22975 (7)	0.19629 (9)	0.0535 (10)
C11*A*	−0.10339 (17)	0.32652 (10)	0.16306 (12)	0.0418 (11)
C12*A*	−0.13097 (19)	0.38478 (11)	0.16821 (13)	0.0500 (13)
C13*A*	−0.04583 (22)	0.41897 (10)	0.16176 (13)	0.0514 (15)
C14*A*	0.03433 (19)	0.38204 (10)	0.15238 (12)	0.0437 (13)
C15*A*	−0.00073 (17)	0.32427 (9)	0.15342 (11)	0.0366 (11)
C1*A*	0.05253 (17)	0.26957 (9)	0.13895 (11)	0.0373 (11)
C21*A*	0.16569 (18)	0.28055 (10)	0.13846 (13)	0.0443 (13)
C22*A*	0.24542 (22)	0.27318 (16)	0.20168 (16)	0.0765 (21)
C23*A*	0.3482 (3)	0.28287 (20)	0.20081 (23)	0.106 (3)
C24*A*	0.3722 (3)	0.29949 (18)	0.1378 (3)	0.093 (3)
C25*A*	0.2946 (3)	0.30684 (17)	0.07551 (21)	0.0865 (24)
C26*A*	0.19089 (22)	0.29750 (15)	0.07545 (16)	0.0692 (19)
C31*A*	−0.00877 (18)	0.24281 (10)	0.06505 (12)	0.0438 (12)
C32*A*	0.00569 (25)	0.18546 (12)	0.05098 (15)	0.0620 (16)
C33*A*	−0.0491 (3)	0.16084 (14)	−0.01549 (20)	0.0816 (24)
C34*A*	−0.1161 (3)	0.19305 (21)	−0.06793 (20)	0.094 (3)
C35*A*	−0.1293 (3)	0.24931 (21)	−0.05547 (18)	0.106 (3)
C36*A*	−0.0761 (3)	0.27397 (15)	0.01084 (16)	0.0783 (19)

Fe2	0.00000	−0.027433 (21)	0.25000	0.0525 (3)
O1*B*	0.08988 (15)	0.11400 (7)	0.22158 (11)	0.0653 (12)
C11*B*	0.01329 (23)	0.00908 (13)	0.15451 (15)	0.0599 (16)
C12*B*	−0.0127 (3)	−0.04931 (15)	0.14299 (19)	0.0785 (22)
C13*B*	0.0677 (3)	−0.08152 (13)	0.19150 (21)	0.0784 (23)
C14*B*	0.14239 (22)	−0.04303 (11)	0.23306 (16)	0.0598 (17)
C15*B*	0.10919 (20)	0.01393 (10)	0.21042 (13)	0.0484 (13)
C1*B*	0.16801 (19)	0.06976 (10)	0.23244 (14)	0.0501 (14)
C21*B*	0.23284 (20)	0.06863 (11)	0.31259 (15)	0.0521 (14)
C22*B*	0.20595 (22)	0.10055 (13)	0.36652 (18)	0.0661 (18)
C23*B*	0.2655 (3)	0.09817 (17)	0.43950 (20)	0.0885 (25)
C24*B*	0.3519 (3)	0.06354 (19)	0.45919 (19)	0.093 (3)
C25*B*	0.3808 (3)	0.03205 (16)	0.40646 (19)	0.0839 (21)
C26*B*	0.32353 (23)	0.03484 (13)	0.33397 (16)	0.0660 (17)
C31*B*	0.23728 (23)	0.08194 (12)	0.18059 (17)	0.0629 (18)
C32*B*	0.3100 (4)	0.12464 (18)	0.1970 (3)	0.111 (3)
C33*B*	0.3743 (5)	0.1361 (3)	0.1509 (4)	0.147 (5)
C34*B*	0.3656 (5)	0.1055 (3)	0.0884 (4)	0.134 (5)
C35*B*	0.2932 (5)	0.0644 (3)	0.0711 (3)	0.132 (4)
C36*B*	0.2293 (3)	0.05215 (18)	0.11698 (22)	0.099 (3)
HO*A*1	0.035	0.235	0.224	0.0642
HO*A*2	0.069	0.206	0.194	0.0642
HO*B*1	0.045	0.108	0.231	0.0770
HO*B*2	0.104	0.142	0.212	0.0770

Table 4. *Summary of dimension ranges* (Å, °) *for* (I)-(III)

	(I)	(II)	(III)
Fe—C_{cp}	2.029(4)-2.053(3)	2.037(2)-2.057(2)	2.033(3)-2.052(2)
Mean	2.043(3)	2.048(2)	2.040(3)
C_{cp}—C_{cp}	1.406(4)-1.425(3)	1.388(3)-1.430(2)	1.405(5)-1.426(3)
Mean	1.419(3)	1.414(3)	1.418(4)
C_{cp}—Csp^3	1.515(3)	1.517(2)	1.516(3), 1.517(3)
Csp^3—Csp^3	1.518(3)	—	—
C_{ar}—Csp^3	1.526(3)	1.533(2)-1.534(2)	1.524(3)-1.543(3)
Csp^3—O	1.441(3)	1.439(2)	1.427(3)-1.438(3)
C_{ar}—C_{ar}	1.362(4)-1.389(3)	1.363(4)-1.398(2)	1.334(10)-1.405(4)
Mean	1.380(3)	1.384(3)	1.374(6)
O—C—Csp^3	108.69(17)	—	—
O—C—C_{ar}	109.46(17)	105.1(1), 110.4(1)	106.0(2)-107.9(2)
O—C—C_{cp}	106.83(17)	109.9(1)	107.9(2),110.4(2)

1-Ferrocenyl-1-phenylethanol (I) was obtained from the reaction of acetylferrocene with phenyllithium, and crystals were grown by slow evaporation of a solution in CH_2Cl_2. Ferrocenyl(diphenyl)methanol (II) was obtained from the reaction of benzoylferrocene with phenyllithium; crystals were obtained by slow evaporation of a solution in CH_2Cl_2. Ferrocene-1,1′-diylbis(diphenylmethanol) (III) was obtained from the reaction of 1,1′-dibenzoylferrocene with phenyllithium; crystals were grown by slow evaporation of a solution in dichloromethane/petroleum (b.p. 313-333 K).

Data collection and cell refinement: Enraf-Nonius CAD-4 software. Data reduction, program used to solve and refine structure, software used to prepare material for publication: *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989).

The space group for (I) was determined unambiguously from the systematic absences (*h*0*l* absent if $h+l = 2n+1$, 0*k*0 absent if $k = 2n+1$) as $P2_1/n$. Molecule (II) crystallized in the triclinic system; space group $P\bar{1}$ was assumed and confirmed by the analysis. The systematic absences for (III) (*hkl* absent if $h+k = 2n+1$, *h*0*l* absent if $l = 2n+1$) allow the space group to be either *C*2/*c* or *Cc*; the former was assumed and confirmed by the analysis. In molecule (I) it was clear from early difference maps that the unsubstituted C_5 ring was disordered over two sites; occupancies of 0.87 and 0.13 were estimated from Fourier and difference Fourier maps. In all three structures, the H atoms attached to the C atoms were clearly visible in difference maps [except for the minor C_5 ring of (I)]; they were positioned geometrically (C—H 0.95 Å) and included as riding atoms in the structure factor calculations. The hydroxyl H atoms [disordered equally in (III) over two sites] were included in the structure factor calculations at the positions obtained from difference maps. The *ORTEP* diagrams were prepared using *ORTEP*II (Johnson, 1976).

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55804 (77 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: L11034]

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Structure of Dimethyl 9-Methyl-9,10-dihydro-9,10-ethenoanthracene-11,12-dicarboxylate

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Abstract

There are two molecules per asymmetric unit and the two ester groups have different orientations in each of them; the C=C—C=O torsion angles are 1.9 and 2.4(6)° for the groups remote from and 91.7 and −91.4(5)° for the

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