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2-Chloro-1-ferrocenylethanol

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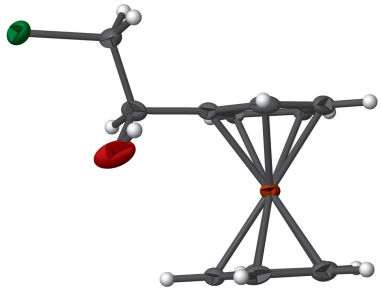
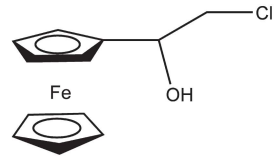
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Fe(C_5H_5)(C_7H_8ClO)]$, the ferrocene cyclopentadiene rings are slightly staggered and inclined to one another at an angle of 0.79 (13)°. In the crystal, C—H···Cl and C—H···O hydrogen bonds each form inversion dimers and these combine with an edge-to-face C—H···π hydrogen bond to stack the molecules along the *b*-axis direction.

3D view



Chemical scheme



Structure description

The title compound $[Fe(C_5H_5)(C_7H_8ClO)]$, (1), Fig. 1, synthesized by the lithium aluminium hydride reduction of 2-chloro-1-ferrocenylethanone, is used in the synthesis of 1,2-dihydroxyethyl ferrocene (Schlögl & Egger, 1963). The two Cp rings of the ferrocene unit are slightly staggered with a mean C···*Cg*1···*Cg*2···C angle of 14.8 (3)° (*Cg*1 and *Cg*2 are the centroids of the substituted and unsubstituted Cp rings, respectively). The rings are almost coplanar with an angle of 0.79 (13)° between them. The methylene C atom lies close to the plane of the substituted Cp ring with the OH and CH_2Cl units of the chloroethanol substituent pointing towards and away from the Fe atom, respectively. In the crystal, three molecules are linked *via* C—H···Cl hydrogen bonds (Table 1), forming two inversion dimers with a third inversion dimer resulting from C—H···O contacts. A C—H···π(ring) hydrogen bond completes the intermolecular interactions that combine to stack chains of molecules along the *b* axis, Fig. 2.

The structures of three other ferrocenylethanol derivatives are known (Glidewell *et al.*, 1996; Pool *et al.*, 1998). The Cambridge Structural Database (Groom & Allen, 2014) also reveals several 1-hydroxyferrocene compounds (Kowalski *et al.*, 2012, 2013; Jary & Baumgartner, 1998; Niazimbetova *et al.*, 1999). We have also recently reported the closely related derivative 2-chloro-1-ferrocenylethanone (McAdam & Simpson, 2016).

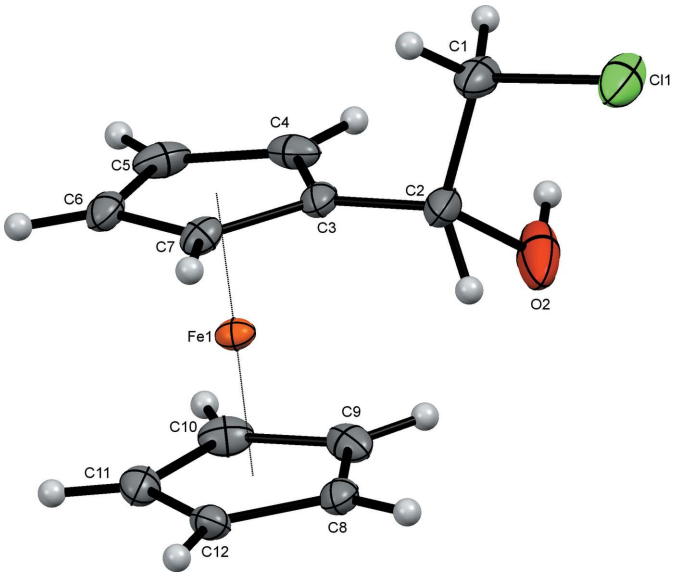


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

Synthesis and crystallization

The title compound was synthesized by a literature method (Schlögl & Egger, 1963). Orange blocks for the X-ray study were grown from a CH_2Cl_2 solution layered with hexane.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. High displacement parameters for the O2 atom and the fact that no hydrogen bond is formed involving this hydroxyl group suggests possible disorder. However, a reasonable disorder model for the H atom bound to O2 could not be developed. Two low-angle reflections with $F_o << F_c$ that may have been affected by the beamstop were omitted from the final refinement cycles.

Acknowledgements

We thank the NZ Ministry of Business, Innovation and Employment Science Investment Fund (grant No. UOO-X1206) for support of this work and the University of Otago for the purchase of the diffractometer. JS thanks the Chemistry Department, University of Otago, for the support of his work.

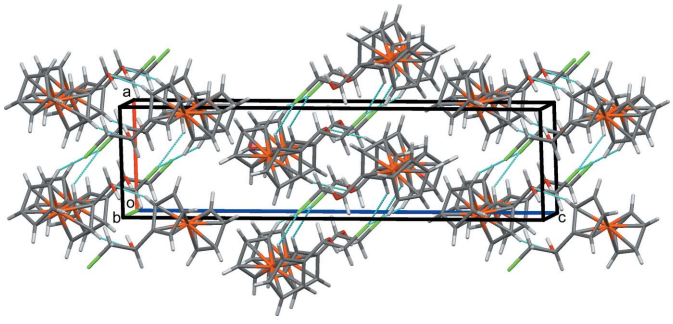


Figure 2
Crystal packing of the title compound, viewed along the *b*-axis direction. Hydrogen bonds are drawn as blue dashed lines.

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

Cg2 is the centroid of the C8–C12 Cp ring.

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O2^{i}	0.95	2.55	3.472 (3)	164
C7—H7···Cl1^{ii}	0.95	2.89	3.6720 (17)	141
C8—H8···Cl1^{iii}	0.95	2.81	3.5153 (17)	132
C12—H12···*Cg2*^{iv}	0.95	2.88	3.6321 (17)	137

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y, -z+1$; (iii) $-x, -y+1, -z+1$; (iv) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Fe(C_5H_5)(C_7H_8ClO)]$
M_r	264.52
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	92
a, b, c (Å)	6.0366 (4), 7.6215 (5), 23.0837 (14)
β (°)	91.737 (3)
V (Å^3)	1061.55 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.64
Crystal size (mm)	0.36 × 0.22 × 0.12
Data collection	
Diffractometer	Bruker APEXII CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2011)
T_{min}, T_{max}	0.805, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19263, 3807, 3355
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.777
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.035, 0.094, 1.03
No. of reflections	3807
No. of parameters	140
No. of restraints	6
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.11, −0.88

Computer programs: *APEX2* (Bruker, 2011), *SAINT* (Bruker, 2011), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *TITAN2000* (Hunter & Simpson, 1999), *Mercury* (Macrae *et al.*, 2008), *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009), *publCIF* (Westrip, 2010).

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full crystallographic data

IUCrData (2016). **1**, x160102 [doi:10.1107/S2414314616001024]

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Crystal data

$[Fe(C_5H_5)(C_7H_8ClO)]$
M_r = 264.52
Monoclinic, $P2_1/n$
a = 6.0366 (4) Å
b = 7.6215 (5) Å
c = 23.0837 (14) Å
β = 91.737 (3)°
V = 1061.55 (12) Å^3
Z = 4
$F(000)$ = 544
D_x = 1.655 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8579 reflections
θ = 2.8–32.3°
μ = 1.64 mm^{-1}
T = 92 K
Block, orange
0.36 × 0.22 × 0.12 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2011)
T_{min} = 0.805, T_{max} = 1.000
19263 measured reflections
3807 independent reflections
3355 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 33.5°, θ_{min} = 3.5°
h = −9→9
k = −9→11
l = −35→35

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.094
S = 1.03
3807 reflections
140 parameters
6 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 1.2107P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.06729 (10)	0.20675 (7)	0.42483 (2)	0.03633 (13)
C1	0.2756 (3)	0.1647 (3)	0.47986 (8)	0.0272 (4)
H1A	0.2822	0.0371	0.4878	0.033*
H1B	0.4218	0.2016	0.4658	0.033*
C2	0.2281 (4)	0.2618 (3)	0.53529 (8)	0.0292 (4)
H2	0.0824	0.2199	0.5494	0.035*
O2	0.2121 (5)	0.4418 (2)	0.52523 (8)	0.0592 (6)
H2A	0.337 (7)	0.449 (6)	0.511 (2)	0.089*
C3	0.4036 (3)	0.2173 (2)	0.58031 (7)	0.0194 (3)
C4	0.6268 (3)	0.2814 (2)	0.58528 (8)	0.0246 (3)
H4	0.6924	0.3656	0.5608	0.029*
C5	0.7325 (3)	0.1961 (3)	0.63363 (9)	0.0255 (4)
H5	0.8811	0.2141	0.6471	0.031*
C6	0.5779 (3)	0.0800 (2)	0.65812 (7)	0.0217 (3)
H6	0.6054	0.0065	0.6908	0.026*
C7	0.3751 (3)	0.0919 (2)	0.62570 (7)	0.0185 (3)
H7	0.2436	0.0280	0.6328	0.022*
Fe1	0.45990 (4)	0.33245 (3)	0.65905 (2)	0.01497 (7)
C8	0.2107 (3)	0.5095 (2)	0.67295 (7)	0.0200 (3)
H8	0.0782	0.5233	0.6501	0.024*
C9	0.4145 (3)	0.5980 (2)	0.66431 (7)	0.0232 (3)
H9	0.4423	0.6809	0.6347	0.028*
C10	0.5702 (3)	0.5403 (2)	0.70817 (8)	0.0240 (3)
H10	0.7197	0.5780	0.7129	0.029*
C11	0.4608 (3)	0.4159 (2)	0.74365 (7)	0.0216 (3)
H11	0.5247	0.3564	0.7762	0.026*
C12	0.2397 (3)	0.3966 (2)	0.72168 (7)	0.0190 (3)
H12	0.1302	0.3215	0.7369	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0448 (3)	0.0318 (2)	0.0313 (2)	0.0146 (2)	−0.0173 (2)	−0.01182 (18)
C1	0.0314 (9)	0.0271 (9)	0.0227 (8)	0.0102 (7)	−0.0066 (7)	−0.0091 (6)
C2	0.0397 (10)	0.0277 (9)	0.0199 (7)	0.0173 (8)	−0.0021 (7)	−0.0005 (7)
O2	0.1191 (15)	0.0275 (8)	0.0296 (7)	0.0287 (9)	−0.0176 (9)	−0.0034 (6)
C3	0.0251 (7)	0.0162 (7)	0.0168 (6)	0.0066 (6)	−0.0008 (5)	−0.0021 (5)
C4	0.0293 (8)	0.0186 (7)	0.0266 (8)	−0.0014 (6)	0.0132 (7)	−0.0049 (6)
C5	0.0155 (7)	0.0283 (9)	0.0327 (9)	0.0017 (6)	0.0008 (6)	−0.0135 (7)
C6	0.0253 (7)	0.0170 (7)	0.0224 (7)	0.0070 (6)	−0.0032 (6)	−0.0028 (6)
C7	0.0187 (6)	0.0131 (6)	0.0236 (7)	0.0002 (5)	−0.0016 (5)	−0.0040 (5)
Fe1	0.01566 (11)	0.01211 (11)	0.01724 (11)	−0.00047 (7)	0.00223 (7)	−0.00292 (7)
C8	0.0238 (7)	0.0178 (7)	0.0182 (7)	0.0059 (6)	−0.0008 (5)	−0.0024 (5)
C9	0.0365 (9)	0.0133 (7)	0.0203 (7)	−0.0018 (6)	0.0071 (6)	−0.0024 (5)
C10	0.0230 (7)	0.0205 (8)	0.0286 (8)	−0.0046 (6)	0.0026 (6)	−0.0097 (6)

C11	0.0258 (7)	0.0205 (7)	0.0181 (7)	0.0025 (6)	−0.0030 (6)	−0.0038 (6)
C12	0.0219 (7)	0.0188 (7)	0.0164 (6)	0.0002 (6)	0.0049 (5)	−0.0007 (5)

Geometric parameters (Å, º)

Cl1—C1	1.7893 (19)	C6—H6	0.9500
C1—C2	1.513 (3)	C7—Fe1	2.0475 (16)
C1—H1A	0.9900	C7—H7	0.9500
C1—H1B	0.9900	Fe1—C9	2.0466 (17)
C2—O2	1.395 (3)	Fe1—C10	2.0476 (17)
C2—C3	1.500 (2)	Fe1—C12	2.0528 (15)
C2—H2	1.0000	Fe1—C8	2.0533 (16)
O2—H2A	0.83 (4)	Fe1—C11	2.0537 (16)
C3—C7	1.433 (2)	C8—C9	1.423 (3)
C3—C4	1.435 (3)	C8—C12	1.423 (2)
C3—Fe1	2.0375 (16)	C8—H8	0.9500
C4—C5	1.426 (3)	C9—C10	1.430 (3)
C4—Fe1	2.0422 (17)	C9—H9	0.9500
C4—H4	0.9500	C10—C11	1.428 (3)
C5—C6	1.416 (3)	C10—H10	0.9500
C5—Fe1	2.0472 (17)	C11—C12	1.421 (2)
C5—H5	0.9500	C11—H11	0.9500
C6—C7	1.418 (2)	C12—H12	0.9500
C6—Fe1	2.0521 (17)		
C2—C1—Cl1	111.45 (13)	C4—Fe1—C6	68.44 (7)
C2—C1—H1A	109.3	C9—Fe1—C6	167.18 (8)
Cl1—C1—H1A	109.3	C5—Fe1—C6	40.43 (8)
C2—C1—H1B	109.3	C10—Fe1—C6	128.61 (7)
Cl1—C1—H1B	109.3	C7—Fe1—C6	40.48 (7)
H1A—C1—H1B	108.0	C3—Fe1—C12	129.56 (7)
O2—C2—C3	112.43 (19)	C4—Fe1—C12	168.29 (8)
O2—C2—C1	110.76 (17)	C9—Fe1—C12	68.39 (7)
C3—C2—C1	109.13 (15)	C5—Fe1—C12	150.03 (8)
O2—C2—H2	108.1	C10—Fe1—C12	68.42 (7)
C3—C2—H2	108.1	C7—Fe1—C12	108.56 (7)
C1—C2—H2	108.1	C6—Fe1—C12	117.60 (7)
C2—O2—H2A	94 (3)	C3—Fe1—C8	108.61 (7)
C7—C3—C4	107.59 (15)	C4—Fe1—C8	129.63 (7)
C7—C3—C2	124.01 (17)	C9—Fe1—C8	40.61 (7)
C4—C3—C2	128.34 (17)	C5—Fe1—C8	167.82 (8)
C7—C3—Fe1	69.85 (9)	C10—Fe1—C8	68.45 (7)
C4—C3—Fe1	69.59 (10)	C7—Fe1—C8	118.11 (7)
C2—C3—Fe1	128.03 (12)	C6—Fe1—C8	150.92 (7)
C5—C4—C3	107.72 (15)	C12—Fe1—C8	40.55 (6)
C5—C4—Fe1	69.79 (10)	C3—Fe1—C11	167.74 (7)
C3—C4—Fe1	69.23 (9)	C4—Fe1—C11	149.86 (8)
C5—C4—H4	126.1	C9—Fe1—C11	68.52 (7)

C3—C4—H4	126.1	C5—Fe1—C11	116.79 (7)
Fe1—C4—H4	126.4	C10—Fe1—C11	40.75 (7)
C6—C5—C4	108.22 (15)	C7—Fe1—C11	128.91 (7)
C6—C5—Fe1	69.97 (10)	C6—Fe1—C11	108.02 (7)
C4—C5—Fe1	69.41 (10)	C12—Fe1—C11	40.50 (7)
C6—C5—H5	125.9	C8—Fe1—C11	68.21 (7)
C4—C5—H5	125.9	C9—C8—C12	108.14 (15)
Fe1—C5—H5	126.3	C9—C8—Fe1	69.44 (10)
C5—C6—C7	108.56 (16)	C12—C8—Fe1	69.71 (9)
C5—C6—Fe1	69.60 (10)	C9—C8—H8	125.9
C7—C6—Fe1	69.59 (9)	C12—C8—H8	125.9
C5—C6—H6	125.7	Fe1—C8—H8	126.5
C7—C6—H6	125.7	C8—C9—C10	107.92 (15)
Fe1—C6—H6	126.7	C8—C9—Fe1	69.95 (10)
C6—C7—C3	107.91 (15)	C10—C9—Fe1	69.60 (10)
C6—C7—Fe1	69.93 (9)	C8—C9—H9	126.0
C3—C7—Fe1	69.09 (9)	C10—C9—H9	126.0
C6—C7—H7	126.0	Fe1—C9—H9	126.0
C3—C7—H7	126.0	C11—C10—C9	107.76 (15)
Fe1—C7—H7	126.5	C11—C10—Fe1	69.86 (9)
C3—Fe1—C4	41.17 (7)	C9—C10—Fe1	69.52 (10)
C3—Fe1—C9	117.38 (7)	C11—C10—H10	126.1
C4—Fe1—C9	107.95 (7)	C9—C10—H10	126.1
C3—Fe1—C5	68.87 (7)	Fe1—C10—H10	126.1
C4—Fe1—C5	40.81 (8)	C12—C11—C10	108.04 (15)
C9—Fe1—C5	128.99 (8)	C12—C11—Fe1	69.72 (9)
C3—Fe1—C10	150.44 (8)	C10—C11—Fe1	69.40 (10)
C4—Fe1—C10	116.66 (7)	C12—C11—H11	126.0
C9—Fe1—C10	40.88 (8)	C10—C11—H11	126.0
C5—Fe1—C10	107.50 (7)	Fe1—C11—H11	126.5
C3—Fe1—C7	41.06 (7)	C11—C12—C8	108.14 (15)
C4—Fe1—C7	68.90 (7)	C11—C12—Fe1	69.78 (9)
C9—Fe1—C7	151.11 (7)	C8—C12—Fe1	69.75 (9)
C5—Fe1—C7	68.39 (7)	C11—C12—H12	125.9
C10—Fe1—C7	166.99 (7)	C8—C12—H12	125.9
C3—Fe1—C6	68.62 (7)	Fe1—C12—H12	126.1

Cl1—C1—C2—O2	−57.5 (2)	C4—C5—C6—C7	−0.22 (19)
Cl1—C1—C2—C3	178.25 (14)	C5—C6—C7—C3	−0.01 (19)
O2—C2—C3—C7	136.5 (2)	C4—C3—C7—C6	0.23 (18)
C1—C2—C3—C7	−100.2 (2)	C2—C3—C7—C6	177.67 (15)
O2—C2—C3—C4	−46.6 (3)	C12—C8—C9—C10	−0.31 (19)
C1—C2—C3—C4	76.7 (2)	C8—C9—C10—C11	0.06 (19)
C7—C3—C4—C5	−0.36 (18)	C9—C10—C11—C12	0.21 (19)
C2—C3—C4—C5	−177.66 (16)	C10—C11—C12—C8	−0.40 (19)
C3—C4—C5—C6	0.36 (19)	C9—C8—C12—C11	0.44 (18)

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C8–C12 Cp ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O2^{i}	0.95	2.55	3.472 (3)	164
C7—H7···Cl1^{ii}	0.95	2.89	3.6720 (17)	141
C8—H8···Cl1^{iii}	0.95	2.81	3.5153 (17)	132
C12—H12···*Cg*2^{iv}	0.95	2.88	3.6321 (17)	137

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*, −*y*, −*z*+1; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+1/2, *y*−1/2, −*z*+3/2.