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1,1′,2,2′,3,3′,4,4′-Octamethylferrocenium 2,5-dibromo-4-hydroxy-3,6-dioxocyclohexa-1,4-dien-1-olate

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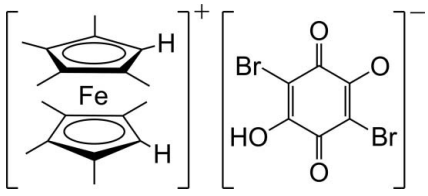
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.084; data-to-parameter ratio = 16.8.

In the title salt, octamethylferrocenium bromanilate, $[Fe(C_9H_{13})_2](C_6HBr_2O_4)$, the Fe atom and the bromanilate anion lie on a mirror plane. The octamethylferrocenium cation adopts an eclipsed conformation. An intramolecular O—H···O hydrogen bond is present in the bromanilate anion. In the crystal, the cations and anions are stacked alternately, forming a one-dimensional columnar structure along [010].

Related literature

For general background to ferrocene-based charge-transfer complexes, see: Miller *et al.* (1994); Mochida *et al.* (2007). For organometallic supramolecular compounds, see: Braga *et al.* (2001); Horikoshi *et al.* (2004). For phase transitions in octa- and decamethylferrocene complexes, see: Mochida *et al.* (2011); Mochida & Yoza (2010). For related structures containing bromanilic acid, see: Mochida (2010); Thomas *et al.* (2009); Tomura & Yamashita (2000); Zaman *et al.* (2001*a*,*b*, 2004). For the structure of the octamethylferrocenium cation, see: Miller *et al.* (1989).



Experimental

Crystal data

$[Fe(C_9H_{13})_2](C_6HBr_2O_4)$
M_r = 595.13
Orthorhombic, *Pnma*
a = 14.7106 (15) Å
b = 10.4938 (11) Å
c = 14.9461 (15) Å
V = 2307.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.15 mm^{-1}
T = 173 K
0.38 × 0.08 × 0.08 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.306, T_{max} = 0.746
14287 measured reflections
2804 independent reflections
1699 reflections with $I > 2\sigma(I)$
R_{int} = 0.087

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.084
S = 1.00
2804 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1···O1	1.01 (8)	1.70 (9)	2.534 (5)	137 (7)

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2444).

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supporting information

Acta Cryst. (2011). E**67**, m1012 [doi:10.1107/S1600536811025499]

1,1′,2,2′,3,3′,4,4′-Octamethylferrocenium 2,5-dibromo-4-hydroxy-3,6-dioxocyclohexa-1,4-dien-1-olate

Tomoyuki Mochida

S1. Comment

Organometallic charge-transfer salts (Miller *et al.*, 1994; Mochida *et al.*, 2007) and organometallic hydrogen-bonded supramolecular compounds (Braga *et al.*, 2001, Horikoshi *et al.*, 2004) have attracted attention mainly from the viewpoints of physical properties and crystal engineering, respectively. This paper reports the crystal structure of the title compound, a charge-transfer salt of octamethylferrocene with bromanilic acid. Bromanilic acid acts as proton donor and electron acceptor, and is useful for building organometallic complexes (Mochida, 2010; Thomas *et al.*, 2009; Tomura & Yamashita, 2000; Zaman *et al.*, 2001*a*, 2004).

The title compound consists of octamethylferrocenium cation and bromanilate anion, which is a deprotonated form of bromanilic acid (Fig. 1). The asymmetric unit contains half of the cation and half of the anion, as the Fe atom and bromanilate anion lie on a mirror plane. The Fe—C(Cp) distances in the cation are 2.072 (3)–2.120 (3) Å (average: 2.102 Å), which is a typical value of the octamethylferrocenium cation (Miller *et al.*, 1989). The C_5HMe_4 groups of the cation adopt an eclipsed conformation and exhibit no disorder. In the anion, the C—O bond length to the deprotonated O atom is shortened compared to that to the protonated O atom [1.234 (6) *versus* 1.337 (6) Å]. In the crystal, the cations and anions are alternately stacked along the *b*-axis to form one-dimensional columns (Fig. 2). There are no intermolecular hydrogen bonds, whereas the bromanilate anion shows an intramolecular O—H···O hydrogen bond (Table 1). The local molecular arrangement closely resembles that of a decamethylferrocene–bromanilate compound (Zaman *et al.*, 2011*b*), although they are not isomorphous. In both crystals, the electronegative atoms (O or Br) of the anion appear to surround the Fe atoms of the cation, leading to the co-planar arrangement of the Fe atoms and the anion planes, as seen in Fig. 2b. In this compound, no O···Br close contacts are seen, in contrast to decamethylferrocene–bromanilate compound, and C—H···Br contacts are observed between the cation and anion (H···Br distance = 3.01 Å).

DSC measurements revealed no traces of phase transitions between 120–400 K, whereas decamethyl- and octamethylferrocene complexes often undergo phase transitions associated with order-disorder of the cyclopentadienyl rings (Mochida *et al.*, 2011; Mochida & Yoza, 2010). An exothermic peak corresponding to decomposition was observed around 408 K.

S2. Experimental

Violet needle crystals of the title compound were grown by slow evaporation of solvent from a 1:1 solution of octamethylferrocene and bromanilic acid in dichloromethane at 223 K. IR (KBr, cm^{-1}): 2919, 1642, 1562, 1368, 1336, 1167, 1030, 957, 790, 553.

S3. Refinement

The hydroxyl H atom was identified in a difference Fourier map and allowed to refine isotropically. Other H atoms were placed at calculated positions and refined in a riding model, with C—H = 0.98 (methyl) and 1.00 (aromatic) Å and with U_{iso}(H) = 1.2(1.5 for methyl)U_{eq}(C).

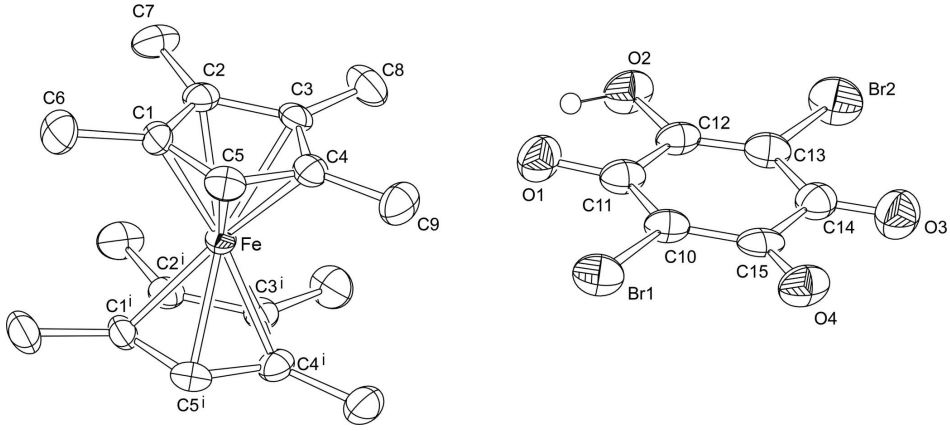

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms except for the hydroxyl group are omitted for clarity. [Symmetry code: (i) x, 1/2-y, z.]

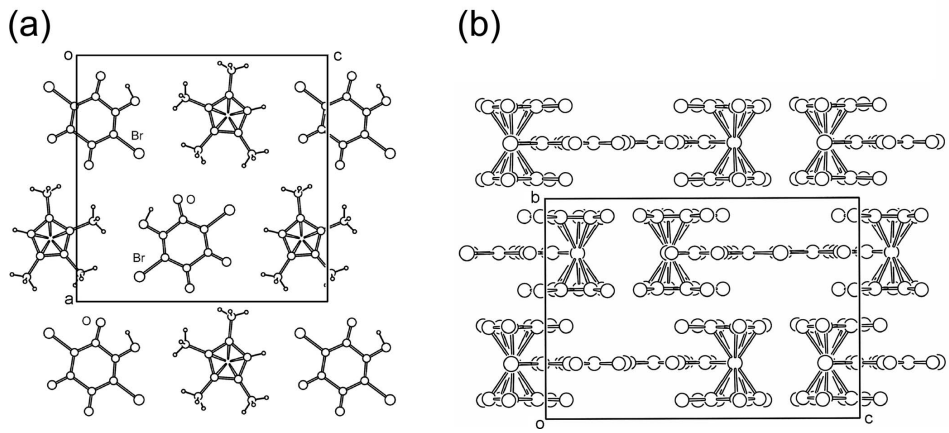

Figure 2

Packing diagrams of the title compound, (a) viewed along the *b*-axis and (b) viewed along the *a*-axis. H atoms are omitted for clarity in (b).

1,1′,2,2′,3,3′,4,4′-Octamethylferrocenium 2,5-dibromo-4-hydroxy-3,6-dioxocyclohexa-1,4-dien-1-olate

Crystal data

$[Fe(C_9H_{13})_2](C_6HBr_2O_4)$
M_r = 595.13
Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
a = 14.7106 (15) Å
b = 10.4938 (11) Å
c = 14.9461 (15) Å
V = 2307.2 (4) Å^3
Z = 4
F(000) = 1196
D_x = 1.713 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 1436 reflections
θ = 2.7–24.0°
μ = 4.15 mm^{-1}
T = 173 K
Needle, violet
0.38 × 0.08 × 0.08 mm

Data collection

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.306, T_{max} = 0.746
14287 measured reflections
2804 independent reflections
1699 reflections with $I > 2\sigma(I)$
R_{int} = 0.087
θ_{max} = 27.5°, θ_{min} = 1.9°
h = −19→18
k = −13→13
l = −19→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.084
S = 1.00
2804 reflections
167 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.032P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.62817 (4)	0.2500	0.60939 (4)	0.04543 (19)
Br2	0.89861 (5)	0.2500	0.25105 (4)	0.0542 (2)
Fe1	0.24413 (4)	0.2500	0.60312 (4)	0.02121 (17)
C2	0.2127 (2)	0.0859 (3)	0.5266 (2)	0.0264 (8)
C1	0.1616 (2)	0.0870 (3)	0.6081 (2)	0.0266 (8)
C5	0.2252 (2)	0.0881 (3)	0.6802 (2)	0.0298 (8)
H5	0.2094	0.0869	0.7453	0.036*
C3	0.3072 (2)	0.0853 (3)	0.5494 (2)	0.0256 (8)
C4	0.3147 (2)	0.0867 (3)	0.6443 (2)	0.0285 (8)
C8	0.3846 (2)	0.0811 (4)	0.4848 (2)	0.0410 (10)
H8A	0.4334	0.1372	0.5058	0.062*
H8B	0.3637	0.1097	0.4259	0.062*
H8C	0.4074	−0.0064	0.4803	0.062*
C7	0.1734 (3)	0.0829 (3)	0.4341 (2)	0.0389 (10)
H7A	0.1633	−0.0057	0.4160	0.058*
H7B	0.2157	0.1236	0.3923	0.058*
H7C	0.1154	0.1288	0.4335	0.058*
C9	0.4003 (2)	0.0809 (4)	0.6978 (3)	0.0420 (10)
H9A	0.4187	−0.0083	0.7052	0.063*
H9B	0.3899	0.1192	0.7567	0.063*
H9C	0.4484	0.1278	0.6666	0.063*
C6	0.0605 (2)	0.0820 (3)	0.6176 (2)	0.0415 (10)
H6A	0.0323	0.1336	0.5705	0.062*
H6B	0.0430	0.1155	0.6763	0.062*

H6C	0.0399	−0.0065	0.6121	0.062*
C12	0.7307 (4)	0.2500	0.3449 (3)	0.0328 (13)
C10	0.7062 (4)	0.2500	0.5083 (3)	0.0324 (13)
C11	0.6678 (4)	0.2500	0.4242 (3)	0.0357 (13)
C15	0.8004 (4)	0.2500	0.5240 (4)	0.0332 (13)
C14	0.8635 (4)	0.2500	0.4391 (4)	0.0365 (13)
C13	0.8211 (4)	0.2500	0.3525 (3)	0.0366 (13)
O1	0.5845 (3)	0.2500	0.4037 (2)	0.0482 (10)
O4	0.8385 (3)	0.2500	0.5975 (2)	0.0473 (11)
O3	0.9454 (3)	0.2500	0.4508 (3)	0.0532 (11)
O2	0.6862 (3)	0.2500	0.2669 (2)	0.0457 (11)
H1	0.625 (5)	0.2500	0.297 (6)	0.13 (3)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0608 (5)	0.0432 (4)	0.0323 (3)	0.000	0.0033 (3)	0.000
Br2	0.0666 (5)	0.0589 (4)	0.0373 (4)	0.000	0.0083 (3)	0.000
Fe1	0.0223 (4)	0.0178 (3)	0.0235 (4)	0.000	−0.0008 (3)	0.000
C2	0.032 (2)	0.0177 (17)	0.030 (2)	−0.0013 (16)	−0.0022 (16)	−0.0020 (15)
C1	0.0208 (18)	0.0214 (18)	0.038 (2)	−0.0037 (14)	0.0036 (16)	0.0001 (17)
C5	0.040 (2)	0.0222 (19)	0.027 (2)	−0.0008 (16)	0.0022 (17)	0.0046 (15)
C3	0.027 (2)	0.0155 (17)	0.034 (2)	0.0029 (15)	0.0043 (15)	−0.0034 (16)
C4	0.031 (2)	0.0206 (19)	0.034 (2)	0.0040 (16)	−0.0047 (16)	−0.0004 (16)
C8	0.038 (3)	0.035 (2)	0.050 (3)	0.0073 (18)	0.0156 (19)	−0.003 (2)
C7	0.055 (3)	0.029 (2)	0.032 (2)	−0.0029 (19)	−0.0125 (18)	−0.0037 (18)
C9	0.040 (2)	0.035 (2)	0.051 (3)	−0.0002 (19)	−0.0165 (19)	0.005 (2)
C6	0.028 (2)	0.036 (2)	0.060 (3)	−0.0081 (18)	0.0086 (19)	0.003 (2)
C12	0.049 (4)	0.026 (3)	0.024 (3)	0.000	−0.010 (3)	0.000
C10	0.049 (4)	0.028 (3)	0.020 (3)	0.000	−0.001 (2)	0.000
C11	0.050 (4)	0.027 (3)	0.030 (3)	0.000	−0.006 (3)	0.000
C15	0.055 (4)	0.014 (3)	0.031 (3)	0.000	−0.006 (3)	0.000
C14	0.041 (4)	0.029 (3)	0.040 (3)	0.000	−0.004 (3)	0.000
C13	0.051 (4)	0.027 (3)	0.032 (3)	0.000	0.001 (3)	0.000
O1	0.046 (3)	0.055 (3)	0.043 (2)	0.000	−0.011 (2)	0.000
O4	0.064 (3)	0.045 (3)	0.033 (2)	0.000	−0.016 (2)	0.000
O3	0.048 (3)	0.060 (3)	0.051 (3)	0.000	−0.006 (2)	0.000
O2	0.060 (3)	0.053 (3)	0.024 (2)	0.000	−0.014 (2)	0.000

Geometric parameters (Å, º)

Br1—C10	1.898 (5)	C8—H8B	0.9800
Br2—C13	1.897 (5)	C8—H8C	0.9800
Fe1—C5^{i}	2.072 (3)	C7—H7A	0.9800
Fe1—C5	2.072 (3)	C7—H7B	0.9800
Fe1—C4^{i}	2.096 (3)	C7—H7C	0.9800
Fe1—C4	2.096 (3)	C9—H9A	0.9800
Fe1—C1^{i}	2.099 (3)	C9—H9B	0.9800

Fe1—C1	2.099 (3)	C9—H9C	0.9800
Fe1—C2^{i}	2.119 (3)	C6—H6A	0.9800
Fe1—C2	2.119 (3)	C6—H6B	0.9800
Fe1—C3^{i}	2.120 (3)	C6—H6C	0.9800
Fe1—C3	2.120 (3)	C12—C13	1.334 (7)
C2—C1	1.432 (4)	C12—O2	1.337 (6)
C2—C3	1.433 (5)	C12—C11	1.505 (7)
C2—C7	1.499 (4)	C10—C11	1.378 (7)
C1—C5	1.427 (5)	C10—C15	1.405 (7)
C1—C6	1.495 (4)	C11—O1	1.262 (6)
C5—C4	1.422 (5)	C15—O4	1.234 (6)
C5—H5	1.0000	C15—C14	1.571 (7)
C3—C4	1.421 (5)	C14—O3	1.218 (6)
C3—C8	1.493 (4)	C14—C13	1.437 (7)
C4—C9	1.493 (4)	O2—H1	1.01 (8)
C8—H8A	0.9800		

C5^{i}—Fe1—C5	110.2 (2)	C1—C5—Fe1	71.03 (19)
C5^{i}—Fe1—C4^{i}	39.90 (13)	C4—C5—H5	125.6
C5—Fe1—C4^{i}	125.03 (14)	C1—C5—H5	125.6
C5^{i}—Fe1—C4	125.03 (14)	Fe1—C5—H5	125.6
C5—Fe1—C4	39.90 (13)	C4—C3—C2	108.2 (3)
C4^{i}—Fe1—C4	109.68 (19)	C4—C3—C8	125.9 (3)
C5^{i}—Fe1—C1^{i}	40.01 (13)	C2—C3—C8	125.9 (3)
C5—Fe1—C1^{i}	124.82 (13)	C4—C3—Fe1	69.39 (19)
C4^{i}—Fe1—C1^{i}	67.03 (14)	C2—C3—Fe1	70.21 (18)
C4—Fe1—C1^{i}	160.47 (14)	C8—C3—Fe1	127.1 (2)
C5^{i}—Fe1—C1	124.82 (13)	C3—C4—C5	107.8 (3)
C5—Fe1—C1	40.00 (13)	C3—C4—C9	126.8 (3)
C4^{i}—Fe1—C1	160.47 (14)	C5—C4—C9	125.4 (3)
C4—Fe1—C1	67.03 (14)	C3—C4—Fe1	71.20 (19)
C1^{i}—Fe1—C1	109.18 (18)	C5—C4—Fe1	69.14 (19)
C5^{i}—Fe1—C2^{i}	66.68 (13)	C9—C4—Fe1	127.5 (2)
C5—Fe1—C2^{i}	159.65 (14)	C3—C8—H8A	109.5
C4^{i}—Fe1—C2^{i}	66.55 (13)	C3—C8—H8B	109.5
C4—Fe1—C2^{i}	158.63 (14)	H8A—C8—H8B	109.5
C1^{i}—Fe1—C2^{i}	39.67 (12)	C3—C8—H8C	109.5
C1—Fe1—C2^{i}	123.73 (13)	H8A—C8—H8C	109.5
C5^{i}—Fe1—C2	159.65 (14)	H8B—C8—H8C	109.5
C5—Fe1—C2	66.68 (13)	C2—C7—H7A	109.5
C4^{i}—Fe1—C2	158.63 (14)	C2—C7—H7B	109.5
C4—Fe1—C2	66.55 (13)	H7A—C7—H7B	109.5
C1^{i}—Fe1—C2	123.73 (13)	C2—C7—H7C	109.5
C1—Fe1—C2	39.68 (12)	H7A—C7—H7C	109.5
C2^{i}—Fe1—C2	108.75 (18)	H7B—C7—H7C	109.5
C5^{i}—Fe1—C3^{i}	66.45 (14)	C4—C9—H9A	109.5
C5—Fe1—C3^{i}	159.74 (13)	C4—C9—H9B	109.5
C4^{i}—Fe1—C3^{i}	39.41 (13)	H9A—C9—H9B	109.5

C4—Fe1—C3^{i}	124.10 (13)	C4—C9—H9C	109.5
C1^{i}—Fe1—C3^{i}	66.56 (13)	H9A—C9—H9C	109.5
C1—Fe1—C3^{i}	158.65 (14)	H9B—C9—H9C	109.5
C2^{i}—Fe1—C3^{i}	39.52 (12)	C1—C6—H6A	109.5
C2—Fe1—C3^{i}	123.65 (14)	C1—C6—H6B	109.5
C5^{i}—Fe1—C3	159.74 (13)	H6A—C6—H6B	109.5
C5—Fe1—C3	66.45 (14)	C1—C6—H6C	109.5
C4^{i}—Fe1—C3	124.10 (13)	H6A—C6—H6C	109.5
C4—Fe1—C3	39.41 (13)	H6B—C6—H6C	109.5
C1^{i}—Fe1—C3	158.65 (14)	C13—C12—O2	124.2 (5)
C1—Fe1—C3	66.56 (13)	C13—C12—C11	123.1 (5)
C2^{i}—Fe1—C3	123.66 (14)	O2—C12—C11	112.7 (5)
C2—Fe1—C3	39.52 (12)	C11—C10—C15	123.9 (5)
C3^{i}—Fe1—C3	109.26 (18)	C11—C10—Br1	118.5 (4)
C1—C2—C3	107.8 (3)	C15—C10—Br1	117.6 (4)
C1—C2—C7	125.7 (3)	O1—C11—C10	128.3 (5)
C3—C2—C7	126.5 (3)	O1—C11—C12	114.0 (5)
C1—C2—Fe1	69.42 (18)	C10—C11—C12	117.8 (5)
C3—C2—Fe1	70.27 (18)	O4—C15—C10	126.6 (5)
C7—C2—Fe1	126.8 (2)	O4—C15—C14	116.8 (5)
C5—C1—C2	107.4 (3)	C10—C15—C14	116.6 (4)
C5—C1—C6	125.5 (3)	O3—C14—C13	123.9 (5)
C2—C1—C6	127.0 (3)	O3—C14—C15	118.0 (5)
C5—C1—Fe1	68.97 (18)	C13—C14—C15	118.1 (5)
C2—C1—Fe1	70.90 (18)	C12—C13—C14	120.6 (5)
C6—C1—Fe1	127.4 (2)	C12—C13—Br2	122.1 (4)
C4—C5—C1	108.8 (3)	C14—C13—Br2	117.4 (4)
C4—C5—Fe1	70.95 (19)	C12—O2—H1	92 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1···O1	1.01 (8)	1.70 (9)	2.534 (5)	137 (7)