P1	0.8999 (9)	0.3125 (9)	0.1192 (7)	0.0170 (10)
P2	0.3218 (10)	0.1185 (9)	0.8729 (7)	0.0170 (10)
P3	0.1411 (10)	0.8546 (9)	0.3311 (7)	0.0170 (10)
F1	0.9192 (21)	0.8875 (19)	0.4878 (14)	0.0228 (15)
O1	0.7149 (25)	0.1209 (21)	0.7279 (17)	0.0228 (15)
O2	0.6609 (26)	0.9471 (23)	0.9697 (18)	0.0228 (15)
O3	0.7682 (24)	0.7471 (22)	0.1386 (18)	0.0228 (15)
O4	0.0354 (25)	0.3027 (22)	0.0368 (17)	0.0228 (15)
O5	0.0722 (24)	0.7623 (24)	0.7350 (19)	0.0228 (15)
O6	0.9613 (26)	0.0273 (22)	0.7321 (18)	0.0228 (15)
O7	0.9291 (25)	0.2953 (24)	0.7220 (18)	0.0228 (15)
O8	0.5223 (26)	0.8249 (22)	0.1495 (18)	0.0228 (15)
O9	0.8055 (25)	0.1458 (23)	0.4969 (19)	0.0228 (15)
O10	0.1199 (24)	0.5246 (22)	0.8592 (18)	0.0228 (15)
O11	0.2641 (26)	0.0150 (24)	0.7495 (18)	0.0228 (15)
O12	0.2408 (26)	0.7476 (23)	0.9864 (18)	0.0228 (15)
C1	0.5505 (64)	0.5414 (56)	0.7447 (43)	0.139 (9)
C2	0.4293 (52)	0.6513 (72)	0.7134 (54)	0.139 (9)
C3	0.5960 (58)	0.7546 (49)	0.5746 (46)	0.139 (9)
C4	0.7256 (50)	0.6670 (57)	0.6562 (50)	0.139 (9)
N1	0.4833 (57)	0.7920 (58)	0.6562 (55)	0.139 (9)
O13	0.6734 (62)	0.5202 (51)	0.6797 (47)	0.139 (9)

Table 2. *Selected geometric parameters* (Å, °)

Al1—O5$^{\rm i}$	1.81 (3)	Al1—O6$^{\rm iv}$	1.87 (2)
Al1—O11$^{\rm ii}$	1.86 (2)	Al1—O9	1.93 (2)
Al1—F1$^{\rm iii}$	1.88 (2)	Al1—F1$^{\rm v}$	1.96 (2)

Al(tetrahedral)—O (mean)	1.72 (2)
Al(tetrahedral)—O (range)	1.69 (2)-1.78 (2)
P—O (mean)	1.53 (2)
P—O (range)	1.46 (2)-1.62 (2)

O5$^{\rm i}$—Al1—O11$^{\rm ii}$	100.4 (10)	F1$^{\rm iii}$—Al1—O9	85.3 (8)
O5$^{\rm i}$—Al1—F1$^{\rm iii}$	92.8 (8)	O11$^{\rm ii}$—Al1—F1$^{\rm v}$	87.0 (10)
O5$^{\rm i}$—Al1—O6$^{\rm iv}$	94.4 (10)	F1$^{\rm iii}$—Al1—F1$^{\rm v}$	79.7 (6)
O11$^{\rm ii}$—Al1—O6$^{\rm iv}$	97.5 (8)	O6$^{\rm iv}$—Al1—F1$^{\rm v}$	84.9 (9)
O5$^{\rm i}$—Al1—O9	92.9 (9)	O9—Al1—F1$^{\rm v}$	86.8 (9)
O11$^{\rm ii}$—Al1—O9	89.5 (9)		

O—Al(tetrahedral)—O (range)	106.4 (10)-112.6 (9)
O—P—O (range)	104.0 (10)-115.2 (13)

Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $1-x, -y, 1-z$; (iii) $2-x, 1-y, 1-z$; (iv) $2-x, -y, 1-z$; (v) $x, y-1, z$; (vi) $x, 1+y, z$; (vii) $1-x, 1-y, 2-z$; (viii) $1-x, 2-y, 1-z$; (ix) $x-1, y, z$; (x) $x, y, z-1$; (xi) $1+x, y, z$; (xii) $x, y, 1+z$.

The crystal was mounted on a strand of glass wool (1 mm long) attached to a stronger glass fibre. Data were recorded on workstation 9.6 at the SRS, Daresbury, England. Crystal to detector distance was 40 mm and the detector angle (2θ) was −28°. Frames of 0.2° were accumulated for 25-35 s at 2 GeV and 187 mA. A collimator of diameter 0.2 mm was used. The incident beam intensity was monitored continuously and intensity data were corrected for decrease with time. The images were processed offline by *MADNES* (Messerschmidt & Pflugrath, 1987) using a profile-fitting procedure characterized by *EVAL* = 6. Data collection, cell refinement and data reduction were performed using *MADNES*. After refinement of the framework, calculation of the difference map revealed the atoms of the template ion as distinct peaks. Assignment of the F site was based on chemical and geometrical grounds as well as spectroscopic evidence and confirmed by refinement of site occupancy. All atoms were refined isotropically with one temperature factor for Al and P, one for framework O and F and another for non-H template atoms (H-atom $U_{\rm iso}$ was 1.2 times this value). In the last cycles of refinement, the template was refined as a rigid body. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*92 (Sheldrick, 1992). Molecular graphics: *DTMM* (Crabbe & Appleyard, 1991). Software used to prepare material for publication: *SHELXL*92.

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Lists of structure factors and H-atom coordinates have been deposited with the IUCr (Reference: LI1095). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Tetracarbonyl[1-phenyl-*N*-(2-pyridylmethylidene)ethylamine-*N*,*N*′]molybdenum(0)

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Abstract

The Mo atom in the title complex, $[Mo(CO)_4(C_{14}H_{14}N_2)]$ (I), is in a distorted octahedral environment. The Mo—C distances *trans* to each N atom [1.944 (5), 1.955 (4) Å] are significantly shorter than those *cis* to both N atoms [2.031 (5), 2.045 (4) Å]. The carbonyl groups *cis* to both N atoms are bent away from the nitrogen-donor ligand with Mo—C—O angles of 172.1 (4) and 173.9 (4)°.

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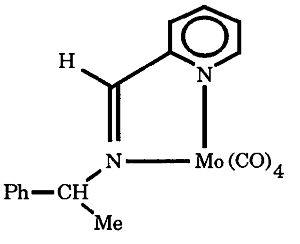
Comment

cis-[M(CO)$_4$(N-N')] complexes (where M = Cr, Mo, W; N-N' = any symmetrical or asymmetrical bidentate nitrogen-donor ligand) are useful starting materials in the synthesis of a variety of N-N'-containing Cr, Mo and W complexes (Kirtley, 1982). Our interest in the reactions of tetracarbonyl[1-phenyl-*N*-(2-pyridylmethylidene)ethylamine-*N*,*N'*]molybdenum(0), (I), whose synthesis has been reported previously (Brunner & Herrmann, 1973), led us to determine its crystal structure. Structures of several such Group 6 complexes have now been established by X-ray diffraction methods; some relevant representative M = Mo cases include tetracarbonyl(azo-2,2'-bipyridine-*N*,*N'*)molybdenum(0) (Kaim, Kohlmann, Jordanov & Fenske, 1991), tetracarbonyl(*N*,*N*-dimethyl-*N'*-benzylethylenediamine)molybdenum(0) (Shiu, Wang & Liao, 1991), tetracarbonyl-[3,6-bis(3,5-dimethylpyrazol-1-yl-N^2)pyridazine-N^2]-molybdenum(0) (Gamasa, Gimeno, Lastra, Garcia-Granda & Morieras, 1991), (*R*)-tetracarbonyl{2-methoxymethyl-1-[(2-pyridyl)methylideneamino]pyrrolidine-*N*,*N'*,*N''*}molybdenum(0), (Ehlers & Dieck, 1988), tetracarbonyl{2,6-[1-(2,2-dimethylpropanimino)ethyl]pyridine-*N*,*N'*}molybdenum(0) (Lu & Selbin, 1987) and tetracarbonyl[(*E*)-5-methylpyridine-2-carboxaldehyde 2'-pyridylhydrazone]molybdenum(0) (Bruce, Cooper, Freeman & McGrath, 1974).



(I)

A view of molecule (I) together with our atomic numbering scheme is shown in Fig. 1. The Mo atom lies at the centre of a slightly distorted octahedron formed by four carbonyl groups and two *cis* N atoms, with *cis* angles at Mo of between 72.81 (12) and 100.51 (15)°; the acute angle N1—Mo—N6 [72.81 (12)°] reflects the small bite of the 1-phenyl-*N*-(2-pyridylmethylidene)ethylamine ligand. Concomitantly, the angles C3—Mo—N6 and C2—Mo—N1 [100.51 (15) and 96.27 (16)°, respectively] are substantially greater than 90°. The sum of the *cis* angles involving Mo and atoms N1, N6, C2 and C3 (the 'equatorial' plane) is 360.1 (2)°. The pyridyl and phenyl rings and the five-membered chelate ring (Mo, N6, C5, C16, N1) are individually planar.

The Mo—N bond lengths [2.240 (3) and 2.251 (3) Å] fall in the range of values found for the related complexes noted above. The two mutually *trans* carbonyl groups have long Mo—C distances [mean 2.038 (7) Å] compared with those that are *trans* to each N atom [mean 1.950 (6) Å]. Lengthening of the Mo—C bond *trans* to a carbonyl group is expected as a result of the strong *trans* influence of the carbonyl group (Appleton, Clark & Manzer, 1973). As a consequence, the *trans* carbonyl groups have shorter C—O bonds [mean 1.137 (7) Å] compared with those *trans* to the N atoms [mean 1.153 (2) Å]. The *trans* carbonyl groups are both bent away from the neutral nitrogen-donor ligand [Mo—C1—O1 173.9 (4)°, Mo—C4—O4 172.1 (4)°] with torsion angles N6—Mo—C1—O1 133.3 (6) and N6—Mo—C4—C4 −146.8 (6)°. The C=N bond length [C5=N6 1.282 (5) Å] can be compared with the coordinated C=N bond length of 1.295 (12) Å in tetracarbonyl{2,6-[1-(2,2-dimethylpropanimino)ethyl]pyridine-*N*,*N'*}molybdenum(0) (Lu & Selbin, 1987).

In the molecular packing, molecules are separated by normal van der Waals contacts; examination of the structure with *PLATON* (Spek, 1992) showed that there were no solvent-accessible voids in the crystal lattice.

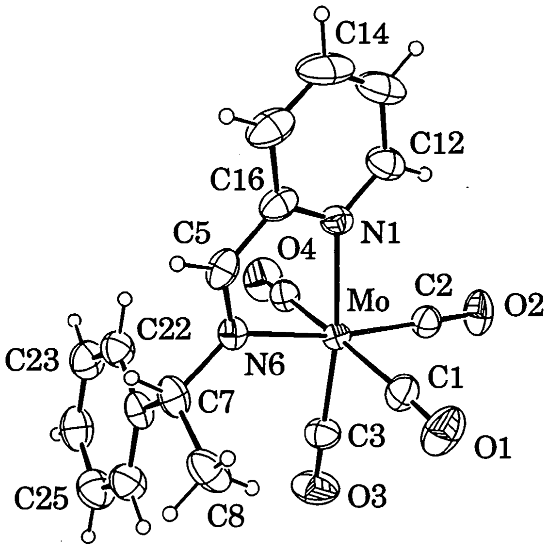


Fig. 1. A view of the tetracarbonyl[1-phenyl-*N*-(2-pyridylmethylidene)-ethylamine-*N*,*N'*]molybdenum(0) molecule. The non-H atoms are shown as displacement ellipsoids drawn at the 35% probability level. For clarity, H atoms are drawn as small spheres of arbitrary size.

Experimental

The complex was synthesized by the reaction of Mo(CO)$_6$ with free ligand in refluxing heptane (Brunner & Herrmann, 1973) and recrystallized from dichloromethane-hexane mixture at 273 K.

Crystal data

[Mo(CO)$_4$(C$_{14}$H$_{14}$N$_2$)] Mo $K\alpha$ radiation
M_r = 418.26 λ = 0.7107 Å

Monoclinic
$P2_1/a$
$a = 13.5889$ (17) Å
$b = 13.752$ (3) Å
$c = 9.7843$ (10) Å
$\beta = 101.785$ (10)°
$V = 1789.9$ (5) Å^3
$Z = 4$
$D_x = 1.552$ Mg m^{-3}

Cell parameters from 25 reflections
$\theta = 6.00$–$22.50°$
$\mu = 0.74$ mm^{-1}
$T = 293$ K
Plate
0.39 × 0.32 × 0.04 mm
Red

Data collection

Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: empirical
$T_{min} = 0.840$, $T_{max} = 0.993$
4050 measured reflections
3896 independent reflections

1978 observed reflections [$I > 3.0\sigma(I)$]
$R_{int} = 0.013$
$\theta_{max} = 26.90°$
$h = -17 \rightarrow 17$
$k = 0 \rightarrow 17$
$l = 0 \rightarrow 12$
3 standard reflections
frequency: 120 min
intensity variation: 1.9%

Refinement

Refinement on F
$R = 0.025$
$wR = 0.031$
$S = 1.00$
1978 reflections
226 parameters
$w = 1/[\sigma^2(F) + 0.0005F^2]$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

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

$U_{eq} = (1/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
Mo	0.25584 (2)	0.49777 (3)	0.37718 (3)	0.04095 (18)
C1	0.1733 (3)	0.3807 (3)	0.4123 (5)	0.061 (3)
O1	0.1285 (3)	0.3114 (3)	0.4212 (5)	0.101 (3)
C2	0.3648 (3)	0.4065 (3)	0.3751 (5)	0.055 (3)
O2	0.4292 (2)	0.3514 (2)	0.3770 (4)	0.083 (2)
C3	0.2050 (3)	0.4768 (3)	0.1776 (4)	0.061 (3)
O3	0.1788 (3)	0.4648 (3)	0.0593 (3)	0.097 (3)
C4	0.3450 (3)	0.6016 (3)	0.3149 (4)	0.054 (3)
O4	0.3966 (3)	0.6513 (3)	0.2701 (4)	0.092 (3)
N1	0.3042 (2)	0.5408 (3)	0.6018 (3)	0.0488 (17)
C12	0.3888 (3)	0.5135 (4)	0.6879 (4)	0.069 (3)
C13	0.4155 (4)	0.5463 (5)	0.8231 (5)	0.092 (4)
C14	0.3535 (6)	0.6052 (5)	0.8743 (5)	0.106 (5)
C15	0.2646 (5)	0.6355 (4)	0.7883 (5)	0.087 (4)
C16	0.2431 (3)	0.6024 (3)	0.6516 (4)	0.059 (3)
C5	0.1545 (3)	0.6334 (3)	0.5512 (5)	0.059 (3)
N6	0.1403 (2)	0.6028 (2)	0.4248 (3)	0.0469 (18)
C7	0.0493 (3)	0.6381 (3)	0.3275 (4)	0.062 (3)
C8	−0.0224 (3)	0.5547 (4)	0.2864 (6)	0.087 (4)
C21	0.0799 (3)	0.6929 (3)	0.2079 (4)	0.054 (2)
C22	0.1557 (3)	0.7612 (4)	0.2364 (5)	0.067 (3)
C23	0.1828 (4)	0.8149 (4)	0.1304 (6)	0.075 (3)
C24	0.1347 (4)	0.8015 (4)	−0.0042 (6)	0.081 (4)
C25	0.0597 (4)	0.7344 (4)	−0.0346 (5)	0.083 (4)
C26	0.0329 (4)	0.6794 (4)	0.0717 (5)	0.073 (3)

Table 2. *Selected geometric parameters* (Å, °)

Mo—C1	2.031 (5)	C14—C15	1.387 (10)
Mo—C2	1.944 (5)	C15—C16	1.387 (6)
Mo—C3	1.955 (4)	C16—C5	1.453 (7)
Mo—C4	2.045 (4)	C5—N6	1.282 (5)
Mo—N1	2.240 (3)	N6—C7	1.480 (5)
Mo—N6	2.251 (3)	C7—C8	1.505 (7)
C1—O1	1.143 (6)	C7—C21	1.519 (6)
C2—O2	1.155 (6)	C21—C22	1.380 (6)
C3—O3	1.151 (5)	C21—C26	1.368 (7)
C4—O4	1.130 (6)	C22—C23	1.383 (7)
N1—C12	1.334 (5)	C23—C24	1.358 (8)
N1—C16	1.345 (6)	C24—C25	1.363 (9)
C12—C13	1.375 (7)	C25—C26	1.392 (7)
C13—C14	1.338 (11)		
C1—Mo—C2	86.45 (18)	C4—Mo—N6	95.40 (14)
C1—Mo—C3	87.54 (19)	N1—Mo—N6	72.81 (12)
C1—Mo—C4	170.18 (18)	Mo—C1—O1	173.9 (4)
C1—Mo—N1	96.02 (16)	Mo—C2—O2	178.3 (4)
C1—Mo—N6	92.37 (15)	Mo—C3—O3	177.3 (4)
C2—Mo—C3	90.52 (18)	Mo—C4—O4	172.1 (4)
C2—Mo—C4	87.07 (17)	Mo—N1—C12	126.0 (3)
C2—Mo—N1	96.27 (16)	Mo—N1—C16	116.3 (3)
C2—Mo—N6	168.85 (15)	C12—N1—C16	117.7 (4)
C3—Mo—C4	85.14 (18)	Mo—N6—C5	115.8 (3)
C3—Mo—N1	172.50 (16)	Mo—N6—C7	127.1 (3)
C3—Mo—N6	100.51 (15)	C5—N6—C7	117.0 (4)
C4—Mo—N1	92.02 (15)		
N1—Mo—C1—O1	−153.7 (7)	N1—Mo—C4—O4	140.2 (6)
N6—Mo—C1—O1	133.3 (6)	N6—Mo—C4—O4	−146.8 (6)

Compound (I) crystallized in the monoclinic system (space group $P2_1/a$ was determined unambiguously by the systematic absences). All non-H atoms were refined by full-matrix least-squares calculations. All H atoms were clearly visible in difference maps; they were positioned geometrically (C—H, N—H 0.95 Å) and included as riding atoms in the structure-factor calculations. Data collection and cell refinement was performed using *CAD*-4 *Software* (Enraf-Nonius, 1989). Data reduction, structure solution and refinement, and preparation of the material for publication were performed using *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989). The diagrams were prepared using *ORTEP*II (Johnson, 1976).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1177). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Hydrogen Bonding in Ferrocene Derivatives: Structures of 1-Ferrocenyl-2,2-dimethylpropan-1-ol and 2,2′-(1,1′-Ferrocenediyl)di(propan-2-ol)

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Abstract

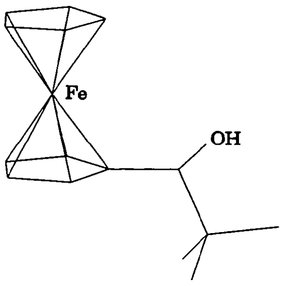
In 1-ferrocenyl-2,2-dimethylpropan-1-ol, $[Fe(C_5H_5)\{(C_5H_4)CH(OH)^tBu\}]$ (I), the molecules are linked by hydrogen bonds to form ribbons around crystallographic 2_1 axes; the O···O distance in the hydrogen bonds is 2.802 (11) Å and the molecules are disordered with *R* and *S* enantiomers occupying common sites. The diol 2,2′-(1,1′-ferrocenediyl)di(propan-2-ol), $[Fe\{(C_5H_4)CMe_2OH\}_2]$ (II), crystallizes as centrosymmetric dimeric aggregates containing fully ordered hydroxyl groups; the dimers are formed by hydrogen bonding, with O···O distances of 2.811 (2) and 2.841 (2) Å.

Comment

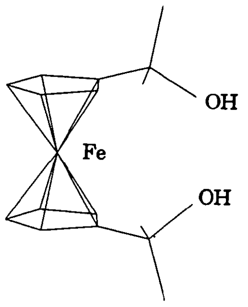
In α-ferrocenyl alcohols of type $[(C_5H_5)Fe\{(C_5H_4)CR'R''OH\}]$ a wide range of O—H···O hydrogen bonding patterns occur in the solid state. Examples have been observed of centrosymmetric dimers containing four-membered $(OH)_2$ rings, as in $Fc_2C(OH)CMe_3$ [Fc = $(C_5H_5)Fe(C_5H_4)$] (Sharma, Cervantes-Lee & Pannell, 1992) and in $FcCPh_2OH$ (Ferguson, Gallagher, Glidewell & Zakaria, 1993), of zigzag chains generated by the action of a glide plane, as in FcCH(OH)Ph (Ferguson, Gallagher, Glidewell & Zakaria, 1994*a*), and of systems with no hydrogen bonding at all, such as FcCMe(OH)Ph (Ferguson, Gallagher, Glidewell & Zakaria, 1993). The relationship between the hydrogen-bonding pattern and the steric and electronic nature of the substituents at the central C atom is, so far, obscure.

In ferrecenediols of type $[Fe\{(C_5H_4)CR'R''OH\}_2]$, on the other hand, there is the possibility either that finite small aggregates may be formed as occurs in, for example, $[(Me_3Si)C]PhSi(OH)_2$ (Aiube, Buttrus, Eaborn, Hitchcock & Zora, 1985), or that chain formation can occur. Examples have been observed where diols form single-stranded chains, as in $[(Me_3Si)_2N]_2Ge(OH)_2$ (Glidewell, Hursthouse, Lloyd, Lumbard & Short, 1986), double-stranded chains, as in $(^tBu)_2Ge(OH)_2$ (Puff, Franken, Schuh & Schwab, 1983), and threefold tubular chains, as in $Ph_2Si(OH)_2$ (Fawcett, Camerman & Camerman, 1977). However, the examples in the ferrocene series which have been examined so far, namely $[Fe\{(C_5H_4)CPh_2OH\}_2]$ (Ferguson, Gallagher, Glidewell & Zakaria, 1993), and racemic $[Fe\{(C_5H_4)CPhMeOH\}_2]$ and $[Fe\{(C_5H_4)CHMeOH\}_2]$ (Ferguson, Gallagher, Glidewell & Zakaria, 1994*b*), have all been found to crystallize as dimers, containing eight-membered $(OH)_4$ rings.

Continuing our systematic study of hydrogen bonding in ferrocene derivatives, we now report the crystal and molecular structures of 1-ferrocenyl-2,2-dimethylpropan-1-ol, $[(C_5H_5)Fe\{(C_5H_4)CH(OH)^tBu\}]$ (I), and 2,2′-(1,1′-ferrocenediyl)di(propan-2-ol), $[Fe\{(C_5H_4)CMe_2OH\}_2]$ (II).



(I)



(II)

Compound (I), Fig. 1, crystallizes in space group $P2_12_12_1$ which would normally accommodate either the *R* or the *S* form resulting from the chiral C atom adjacent to the ferrocenyl group. However, in the crystal structure, the hydroxyl group and the H atom bonded to this stereogenic C atom are disordered over two shared sites and hence both *R* and *S* forms are present. The site occupancies of the O atoms at the two sites consistently refined to 0.65 (1) and 0.35 (1); when the occupancies were constrained to be equal, the isotropic temperature factors attained unacceptable values. Hence, in the crystal selected for analysis there is an excess of one enantiomer over the other, and