C35	−0.1967 (3)	−0.0605 (2)	0.8125 (3)	0.0503 (8)
C36	−0.1259 (4)	−0.1355 (2)	0.7797 (3)	0.0638 (10)
C37	−0.1318 (3)	−0.1370 (3)	0.6701 (3)	0.0643 (10)
C38	−0.2068 (3)	−0.0618 (3)	0.6334 (3)	0.0584 (9)

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

Fe1—C1	2.044 (3)	C1—C5	1.429 (5)
Fe1—C2	2.039 (3)	C1—C11	1.506 (5)
Fe1—C3	2.027 (3)	C2—C12	1.502 (5)
Fe1—C4	2.033 (3)	C3—C13	1.502 (5)
Fe1—C5	2.041 (3)	C4—C14	1.520 (5)
Fe1—C22	2.025 (3)	C5—C15	1.510 (5)
Fe1—C23	2.018 (3)	C21—C22	1.438 (4)
Fe1—C24	2.038 (3)	C21—C28	1.441 (4)
Fe1—C25	2.128 (3)	C21—C25	1.476 (4)
Fe1—C21	2.114 (3)	C22—C23	1.417 (5)
Fe2—C21	2.115 (3)	C23—C24	1.414 (5)
Fe2—C25	2.127 (3)	C24—C25	1.440 (4)
Fe2—C26	2.031 (3)	C25—C26	1.437 (4)
Fe2—C27	2.024 (3)	C26—C27	1.405 (5)
Fe2—C28	2.030 (3)	C27—C28	1.418 (5)
Fe2—C31	2.057 (3)	C31—C35	1.414 (5)
Fe2—C35	2.059 (3)	C31—C38	1.425 (5)
Fe2—C36	2.049 (4)	C31—C32	1.466 (5)
Fe2—C37	2.031 (3)	C32—C33	1.379 (5)
Fe2—C38	2.049 (3)	C33—C34	1.436 (6)
C1—C2	1.412 (5)	C34—C35	1.492 (5)
C2—C3	1.424 (4)	C35—C36	1.411 (5)
C3—C4	1.414 (4)	C36—C37	1.406 (5)
C4—C5	1.394 (5)	C37—C38	1.439 (5)
C2—C1—C5	107.2 (3)	C23—C24—C25	106.9 (3)
C2—C1—C11	126.4 (4)	C26—C25—C24	145.8 (3)
C5—C1—C11	126.3 (4)	C26—C25—C21	106.8 (3)
C1—C2—C3	108.1 (3)	C24—C25—C21	107.4 (3)
C1—C2—C12	126.7 (3)	C27—C26—C25	107.9 (3)
C3—C2—C12	125.2 (3)	C26—C27—C28	110.6 (3)
C4—C3—C2	107.6 (3)	C27—C28—C21	107.0 (3)
C4—C3—C13	126.4 (3)	C35—C31—C38	108.1 (3)
C2—C3—C13	125.9 (3)	C35—C31—C32	109.6 (3)
C5—C4—C3	108.4 (3)	C38—C31—C32	142.4 (3)
C5—C4—C14	126.1 (3)	C33—C32—C31	105.6 (3)
C3—C4—C14	125.5 (3)	C32—C33—C34	113.2 (4)
C4—C5—C1	108.6 (3)	C33—C34—C35	104.2 (3)
C4—C5—C15	126.0 (4)	C36—C35—C31	108.9 (3)
C1—C5—C15	125.4 (4)	C36—C35—C34	143.7 (4)
C22—C21—C28	145.3 (3)	C31—C35—C34	107.4 (3)
C22—C21—C25	107.3 (3)	C37—C36—C35	107.6 (3)
C28—C21—C25	107.4 (3)	C36—C37—C38	108.8 (3)
C23—C22—C21	107.0 (3)	C31—C38—C37	106.6 (3)
C24—C23—C22	111.0 (3)		

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ZORTEP* (Zsolnai & Pritzkow, 1995) and *PLUTON*93 (Spek, 1993). Software used to prepare material for publication: *PARST*95 (Nardelli, 1995) and *PLATON*92 (Spek, 1992).

The authors thank the CEE (project CI1-CT91-0913), the DGICYT (project PB92-0594), the FONDECYT (project 1930024) and DICYT (project 02-9542 CHM) for financial support. The X-ray measurements were carried out at the Servei de Difracció de Raigs-X de la Universitat Autònoma de Barcelona.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1233). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Bunel, E. E., Valle, L., Jones, N. L., Carroll, P. J., Barra, C., González, M., Muñoz, N., Aizman, A. & Manríquez, J. M. (1988). *J. Am. Chem. Soc.* **110**, 6596–6598.

Churchill, M. R. & Lin, K.-K. G. (1973). *Inorg. Chem.* **12**, 2274–2279.

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

Enraf–Nonius (1989). *CAD*-4 *Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.

Howard, J. A. K., Knox, S. A. R., Riera, V., Stone, F. G. A. & Woodward, P. (1974). *J. Chem. Soc. Chem. Commun.* pp. 452–453.

Howard, J. A. K., Knox, S. A. R., Stone, F. G. A., Szary, A. C. & Woodward, P. (1974). *J. Chem. Soc. Chem. Commun.* pp. 788–789.

Howard, J. A. K., Stansfield, R. F. D. & Woodward, P. (1979). *J. Chem. Soc. Dalton Trans.* pp. 1812–1818.

Howard, J. A. K. & Woodward, P. (1978). *J. Chem. Soc. Dalton Trans.* pp. 412–416.

Kitano, Y., Kashiwagi, M. & Kinoshita, Y. (1973). *Bull. Chem. Soc. Jpn*, **46**, 723–727.

Manríquez, J. M., Ward, M. D., Reiff, W. M., Calabrese, J. C., Jones, N. L., Carroll, P. J., Bunel, E. E. & Miller, J. S. (1995). *J. Am. Chem. Soc.* **117**, 6182–6193.

Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Oelckers, B., Chávez, I., Manríquez, J. M. & Román, E. (1993). *Organometallics*, **12**, 3396–3397.

Sheldrick, G. M. (1985). *SHELXS*86. *Crystallographic Computing* 3, edited by G. M. Sheldrick, C. Krüger & R. Goddard, pp. 175–189. Oxford University Press.

Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Spek, A. L. (1992). *PLATON*92. *Program for the Automated Analysis of Molecular Geometry*. University of Utrecht, The Netherlands.

Spek, A. L. (1993). *PLUTON*93. *Program for the Display and Analysis of Crystal and Molecular Structures*. University of Utrecht, The Netherlands.

Stezowski, J. J., Hoier, H., Wilhelm, D., Clark, T. & Schleyer, P. von R. (1985). *J. Chem. Soc. Chem. Commun.* pp. 1263–1264.

Zsolnai, L. & Pritzkow, H. (1995). *ZORTEP*. University of Heidelberg, Germany.

Acta Cryst. (1996). C**52**, 2757–2760

(*SS**,1*S**,2*R**)-1-(Hydroxymethyl)-2-(*p*-tolylsulfinyl)ferrocene

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(*Received 12 July 1996; accepted 30 July 1996*)

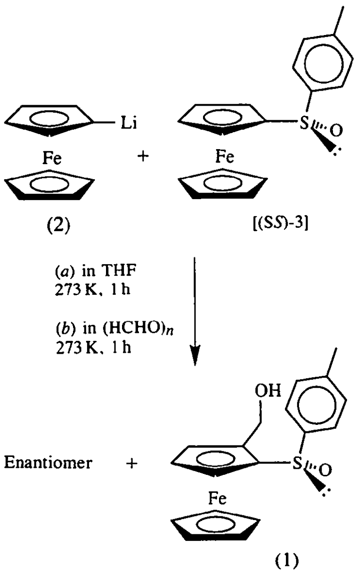
Abstract

The title compound, (*SS**,1*S**,2*R**)-[2-(*p*-tolylsulfinyl)-1-ferrocenyl]methanol, $[Fe(C_{13}H_{13}O_2S)(C_5H_5)]$, isolated as a racemic mixture, was synthesized *via* the rapid

racemization/stereoselective deprotonation of (*SS*)-(*p*-tolylsulfinyl)ferrocene with lithiated ferrocene, followed by reaction with paraformaldehyde. The two cyclopentadienyl rings are almost eclipsed and are tilted at an angle of 5.1 (4)° with respect to one another. Hydrogen bonding between sulfoxide O atoms and hydroxyl H atoms produces infinite one-dimensional molecular chains.

Comment

In our studies of the stereoselective synthesis of bi- and tridentate ferrocenes with S-containing substituents and their use in asymmetric catalysis, we found an interesting racemization of a chiral sulfinyl moiety and, subsequently, an addition reaction with paraformaldehyde which was regioselective. The title compound, (1), was isolated as a single racemic diastereomer in 69% yield from the reaction of (*SS*)-(*p*-tolylsulfinyl)ferrocene, [(*SS*)-3], with lithiated ferrocene, (2), in THF at 273 K for 1 h, followed by reaction with paraformaldehyde. No other diastereomers of (1) were detected in the crude reaction mixture. In the previously reported synthesis of 2-substituted chiral ferrocenyl sulfoxides (Rebiere, Riant, Ricard & Kagan, 1993), racemization of neither the products nor the starting sulfoxide was mentioned. These conflicting results, along with the difficulty in assigning the relative stereochemistry of [(±)-1], prompted us to study the structure of (1) by single-crystal X-ray analysis.



The relative stereochemistry of (1) was established as the *SS**,1*S**,2*R** configuration. The racemization process is believed to result from nucleophilic attack by lithiated ferrocene on the S atom of [(*SS*)-3] to provide [(*SR*)-3] and the ferrocene anion, which is a reversible reaction. At a slower rate, regioselective deprotonation of racemized (3) by lithiated ferrocene subsequently occurs to give the lithiated anion (at the C-1*S** position) in which the lithium ion is chelated with the sulfinyl O atom. Subsequent nucleophilic addition of the lithiated C-1 anion of (3) to paraformaldehyde generates [(±)-1].

Compound (1) crystallized from ether–hexane solution as a racemic mixture. The mean C—C bond distances for the top and bottom cyclopentadienyl rings (Fig. 1) are 1.416 (9) and 1.399 (11) Å, respectively, and the mean Fe—C distance is 2.032 (7) Å. The S1—O1 and C2—C3 bonds of 1.502 (5) and 1.415 (9) Å, respectively, are longer than the corresponding bonds found in 2-methylferrocenyl *tert*-butyl sulfoxide, which were reported as 1.492 (6) and 1.371 (9) Å by Rebiere *et al.* (1993). The distances from the Fe atom to the centroids of the cyclopentadienyl rings (*Cg*1 and *Cg*2) are 1.634 (3) for Fe—*Cg*1 and 1.650 (3) Å for Fe—*Cg*2, with a *Cg*1—Fe—*Cg*2 angle of 175.77 (15)°; the Fe···C11 distance is 3.150 (3) Å. The C2—S1—C12 angle of 100.1 (3)° is the same as that determined for C—S—C in dimethyl sulfoxide (100°; Bastiansen & Viervoll, 1948). The mean value of the five torsion angles from C1—*Cg*1—*Cg*2—C6 through to C5—*Cg*1—*Cg*2—C10 is 6.5 (5)°, indicating that the two cyclopentadienyl rings are close to being mutually eclipsed, which is in agreement with observations for other monosubstituted ferrocenes (Ferguson, Glidewell & Scott, 1995). The angle of 5.1 (4)° between the two cyclopentadienyl ring planes, however, shows that the two rings are not parallel.

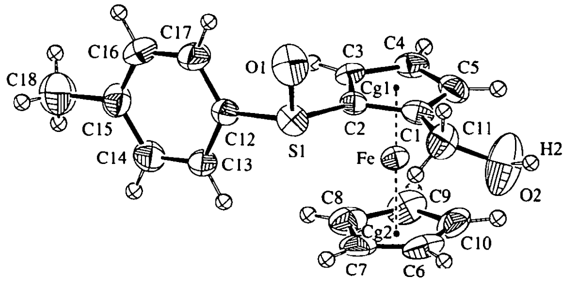


Fig. 1. The molecular configuration and atom numbering scheme for (1), with displacement ellipsoids at the 50% probability level. The centroids of the cyclopentadienyl rings are labeled *Cg*1 and *Cg*2. The H atoms are shown as isotropic spheres of arbitrary radii.

Hydrogen bonding between the H2 atom of the hydroxy group and the O1 atom of the sulfinyl function of an adjacent molecule related by a 2_1 screw transformation leads to infinite one-dimensional molecular chains extending in the **b** direction.

Experimental

The reaction of ferrocene with *tert*-butyllithium in THF at 273 K followed by the addition of (*SS*)-1-menthyl *p*-toluenesulfinate at 195 K over 2 h provided (*SS*)-(*p*-tolylsulfinyl)-ferrocene, [(*SS*)-3], in 55% yield; $[\alpha]_D^{22} = +246°$, indicating an 81% enantiomeric excess (ee) [calculated from the rotation of −305° for the 99% ee of *R* enantiomer reported by Diter, Samuel, Taudien & Kagan (1994)]. A solution of *tert*-butyllithium (0.56 ml, 0.96 mmol; 1.7 *M* in pentanes) was added to a cold (273 K) solution of ferrocene (0.208 g, 1.12 mmol) in 2 ml THF under argon and the mixture stirred for 2 h. A cold (273 K) solution of [(*SS*)-3] (0.26 g, 0.8 mmol) in 2 ml THF was then added. After this mixture was stirred for 1 h, it was cannulated into a cold (273 K) solution of paraformaldehyde (30 mg, 0.96 mmol) in 2 ml THF and the mixture stirred for 1 h. Brine was then added, the mixture extracted with methylene chloride (three times) and the combined extracts dried ($MgSO_4$), concentrated and column chromatographed on silica gel with hexane and ether as eluants, to give 70 mg of (1) [69% yield based on the isolation of almost racemic (3)] and 167 mg (64% isolation) of almost racemic (3). Recrystallization of (1) from a mixture of ether and hexane gave crystals (m.p. 325–327 K) suitable for X-ray analysis.

Crystal data

$[Fe(C_{13}H_{13}O_2S)(C_5H_5)]$
$M_r = 354.25$
Monoclinic
$P2_1/c$
$a = 7.9286\ (16)$ Å
$b = 9.7444\ (14)$ Å
$c = 20.756\ (3)$ Å
$\beta = 93.173\ (14)°$
$V = 1601.2\ (5)$ Å^3
$Z = 4$
$D_x = 1.4695\ (5)$ Mg m^{-3}
D_m not measured

Mo *Kα* radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 7.52–8.48°$
$\mu = 1.068$ mm^{-1}
$T = 296$ K
Plate
0.27 × 0.23 × 0.06 mm
Brown

Data collection

Rigaku AFC-5*S* diffractometer
ω scans (rate 3° min^{-1} in *ω*, maximum of three repetitions)
Absorption correction: empirical *via ψ* scans (North, Phillips & Mathews, 1968)
$T_{min} = 0.83$, $T_{max} = 0.94$
3240 measured reflections
3010 independent reflections

1541 observed reflections $[I > 1.5\sigma(I)]$
$R_{int} = 0.054$
$\theta_{max} = 25°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 11$
$l = -24 \rightarrow 24$
3 standard reflections monitored every 100 reflections
intensity decay: 0.2%

Refinement

Refinement on *F*
$R = 0.058$
$wR = 0.047$
$S = 1.19$
1541 reflections
202 parameters
H atoms riding (C—H 0.95 Å) and H2 coordinates refined
$w = 4F_o^2/\sigma^2(F_o^2)$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.3.1)

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

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

	x	*y*	*z*	U_{eq}
Fe	0.36662 (11)	0.30985 (10)	0.41085 (4)	0.0311 (3)
S1	0.3708 (2)	0.5610 (2)	0.29594 (8)	0.0414 (6)
O1	0.2473 (6)	0.6734 (5)	0.2781 (2)	0.0603 (19)
O2	0.0024 (8)	0.2025 (8)	0.3160 (3)	0.106 (3)
C1	0.1604 (8)	0.3866 (7)	0.3617 (3)	0.036 (2)
C2	0.2954 (7)	0.4834 (6)	0.3661 (3)	0.031 (2)
C3	0.3369 (8)	0.5122 (6)	0.4319 (3)	0.034 (2)
C4	0.2297 (8)	0.4336 (7)	0.4690 (3)	0.040 (2)
C5	0.1211 (8)	0.3565 (7)	0.4255 (3)	0.044 (3)
C6	0.4103 (10)	0.1305 (8)	0.3658 (4)	0.055 (3)
C7	0.5505 (10)	0.2173 (7)	0.3614 (4)	0.054 (3)
C8	0.6122 (9)	0.2473 (8)	0.4240 (4)	0.054 (3)
C9	0.5115 (10)	0.1788 (8)	0.4668 (3)	0.054 (3)
C10	0.3861 (10)	0.1068 (7)	0.4316 (4)	0.055 (3)
C11	0.0775 (8)	0.3294 (8)	0.3009 (3)	0.050 (3)
C12	0.5561 (8)	0.6461 (7)	0.3304 (3)	0.035 (2)
C13	0.7095 (8)	0.5799 (7)	0.3339 (3)	0.047 (3)
C14	0.8498 (9)	0.6500 (8)	0.3570 (4)	0.053 (3)
C15	0.8437 (9)	0.7858 (8)	0.3762 (3)	0.048 (3)
C16	0.6894 (10)	0.8488 (7)	0.3709 (4)	0.056 (3)
C17	0.5450 (9)	0.7810 (7)	0.3476 (4)	0.054 (3)
C18	1.0000 (10)	0.8617 (10)	0.4015 (4)	0.082 (4)
*Cg*1†	0.2287 (3)	0.4345 (3)	0.41084 (13)	
*Cg*2†	0.4941 (4)	0.1761 (3)	0.40992 (17)	

† *Cg*1 and *Cg*2 are the centroids of the C1–C5 and C6–C10 cyclopentadienyl rings, respectively.

Table 2. *Selected geometric parameters (Å, °) and hydrogen-bonding geometry (Å, °)*

Fe—*Cg*1	1.634 (3)	O2—C11	1.415 (11)
Fe—*Cg*2	1.650 (3)	C2—C3	1.415 (9)
S1—O1	1.502 (5)	C1—C11	1.498 (9)
S1—C2	1.774 (6)	C15—C18	1.512 (11)
S1—C12	1.800 (7)		
*Cg*1—Fe—*Cg*2	175.77 (15)	C2—C1—C11	126.4 (6)
O1—S1—C2	105.6 (3)	C5—C1—C11	127.2 (6)
O1—S1—C12	105.6 (3)	O2—C11—C1	108.0 (5)
C2—S1—C12	100.1 (3)	S1—C12—C13	120.3 (5)
S1—C2—C1	121.0 (5)	S1—C12—C17	118.9 (5)
S1—C2—C3	129.6 (5)		

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.88 (9)	1.89 (9)	2.718 (8)	157 (9)

Symmetry code: (i) $-x, y - \frac{1}{2}, \frac{1}{2} - z$.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN PROCESS* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *TEXSAN LS*. Molecular graphics: *ORTEP* (Johnson, 1965). Software used to prepare material for publication: *TEXSAN FINISH* and *PLATON* (Spek, 1990).

DHH thanks the Research Corporation and the National Science Foundation, EPSCoR program, for financial support of this project. We thank Dr Cal Y. Meyers for his help in the preparation of this manuscript.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: FG1218). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Bastiansen, O. & Viervoll, H. (1948). *Acta Chem. Scand.* **2**, 702–706.
Diter, P., Samuel, O., Taudien, S. & Kagan, H. B. (1994). *Tetrahedron Asymm.* **5**, 549–552.
Ferguson, G., Glidewell, C. & Scott, J. P. (1995). *Acta Cryst.* C**51**, 1989–1991.
Johnson, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.
Molecular Structure Corporation (1985). *TEXSAN. TEXRAY Structure Analysis Package*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Molecular Structure Corporation (1988). *MSC/AFC Diffractometer Control Software*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Rebiere, F., Riant, O., Ricard, L. & Kagan, H. B. (1993). *Angew. Chem. Int. Ed. Engl.* **32**, 568–570.
Sheldrick, G. M. (1985). *SHELXS86. Crystallographic Computing* 3, edited by G. M. Sheldrick, C. Krüger & R. Goddard, pp. 175–189. Oxford University Press.
Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.

Acta Cryst. (1996). C**52**, 2760-2763

Hydrogen Bis[(8-quinolinol-*N*)(8-quinolinolato-*N*,*O*)(triphenylphosphine-*P*)silver(I)] Acetate Monohydrate

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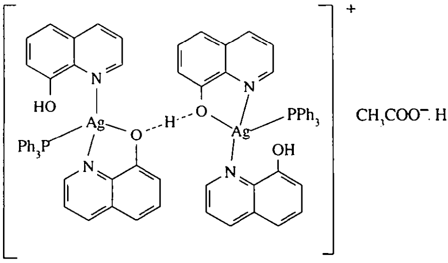
(*Received 11 December 1995; accepted 26 June 1996*)

Abstract

The asymmetric unit of the title compound, $[Ag_2H(C_9H_6NO)_2(C_9H_7NO)_2(C_{18}H_{15}P)_2](C_2H_3O_2).H_2O$, contains two exactly centrosymmetric $[QHQ]^+$ complex cations, $Q = [Ag(PPh_3)(C_9H_6NOH)(C_9H_6NO)]$. The two electroneutral silver complex units, Q, in each cation are connected by a short hydrogen bond [O···O 2.452 (5) and 2.463 (6) Å], with the proton lying at an inversion center. Each Ag atom has a distorted tetrahedral environment, bonding to two quinoline ligands and a PPh_3 ligand; both O and N atoms of the anionic quinolinol ligand are attached to the Ag atom, while in the neutral quinolinol ligand, the bonding is only through the N atom. The fourth coordination site is occupied by the P atom of a PPh_3 ligand. Some differences in the coordination of the two independent Ag atoms are observed. The $[QHQ]^+$ complex cations are linked by the trapped acetate ions through hydrogen bonding which also connects the water molecule to one of the acetate O atoms. In each $[QHQ]^+$ cation, there are intramolecular contacts between the Ag and the phenolic O atom of the neutral quinolinol moieties [Ag···O 2.827 (4) and 2.901 (4) Å].

Comment

Crystallographic studies on $AgL(LH)$, L = 8-hydroxyquinolinate, show the existence of short O···H···O′ hydrogen bonds [O···O 2.457 Å] between adjacent molecules (Fleming & Lynton, 1968). In $Cu^{II}L_2$, a dimeric structure is found with the Cu atom forming a fifth bond to the O atom of a centrosymmetrically related molecule (Cu—O 2.830 Å; Palenik, 1964). The structural study of the title complex, (1), continues our exploration of the reactions of the dimeric binuclear complex, bis[acetato(triphenylphosphine)silver(I)] (Ng & Othman, 1995; Othman, Fun & Sivakumar, 1996).



(1)

An interesting feature of compound (1) is the structure of the $[QHQ]^+$ cation. A displacement ellipsoid plot of one of the two independent Q residues, which have a common numbering scheme, is shown in Fig. 1. In each cation, equivalent Q residues are connected by a short hydrogen bond [O1*A*···O1*A*^{i} 2.452 (5) and O1*B*···O1*B*^{ii} 2.463 (6) Å; symmetry codes: (i) $-x+1$, $-y+2$, $-z+1$; (ii) $-x$, $-y+2$, $-z+1$]. In each case, the proton lies on a center of inversion. Inspection of the atomic coordinates of the two independent Q residues, A and B, revealed the existence of the pseudo-symmetry relationships $x_B \simeq \frac{1}{2} - x_A$ and $y_B \simeq y_A$, the z coordinates being independent. The structure of compound (1) bears significant resemblence to that of hydrogen bis(1-methyl-2-quinolone) hexafluoroarsenate(V), where there is a similar short contact involving a hydrogen bond between the two quinolone moieties [O···O 2.439 (12) Å;

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