Data collection: *CAD-4/PC* (Enraf–Nonius, 1994). Cell refinement: *CAD-4/PC*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1985, 1992). Program(s) used to solve structure: *SIR*92 (Altomare, Cascarano, Giacovazzo & Guagliardi, 1993). Program(s) used to refine structure: *TEXSAN*. Software used to prepare material for publication: *TEXSAN*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: TA1112). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Alegría, A. E., Cox, O., Santiago, V., Colón, M., Reyes, Z., Rivera, L. A. & Dumas, J. A. (1993). *Free Rad. Biol. Med.* **15**, 49–56.
Altomare, A., Cascarano, M., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Cox, O., Jackson, H., Vargas, V. A., Báez, A., Colón, J. I., González, B. C. & De Leon, M. (1982). *J. Med. Chem.* **25**, 1378–1380.
Enraf–Nonius (1994). *CAD-4/PC*. Version 1.5. Enraf–Nonius, Delft, The Netherlands.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Molecular Structure Corporation (1985, 1992). *TEXSAN. TEXRAY Structure Analysis Package*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

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(Z)-2-Acetoxy-3,3′,4′-trimethoxystilbene

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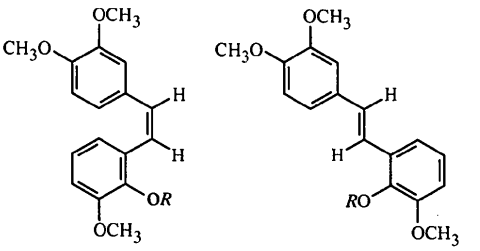
Abstract

The crystal structure determination demonstrates unambiguously that the title compound, 2-[(*Z*)-3,4-dimethoxyphenylethenyl]-6-methoxypheenyl acetate, $C_{19}H_{20}O_5$, has the *Z* configuration. The title compound was prepared by decarboxylation of (*E*)-3-(2-acetoxy-3-methoxyphenyl)-2-(3,4-dimethoxyphenyl)propenoic acid; this compound was in turn obtained by condensation of 2-acetoxy-3-methoxybenzaldehyde with (3,4-dimethoxyphenyl)acetic acid. ^{1}H NMR data for the title compound and the isomeric (*E*)-2-acetoxy-3,3′,4′-trimethoxystilbene are reported.

Comment

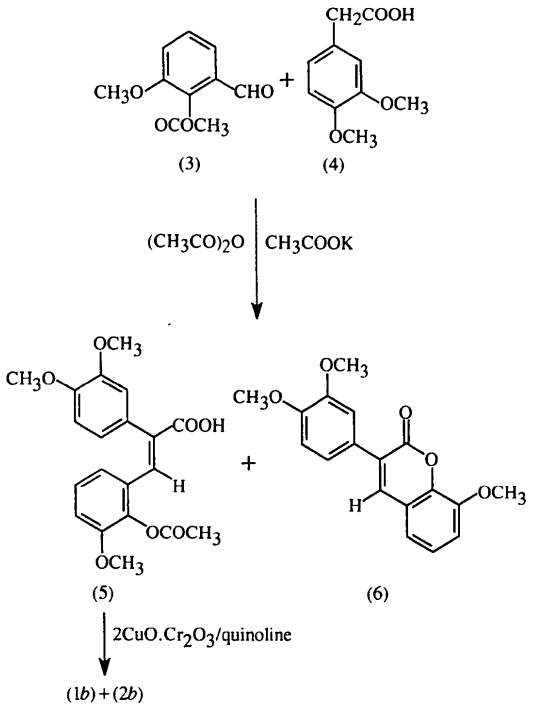
Structural elements in lignins of the phenylcoumaran type are converted into stilbene structures during alkaline pulping (Adler, Marton & Falkehag, 1964; Gierer, Lenic, Norén & Szabo-Lin, 1974; Gierer, Pettersson & Szabo-Lin, 1974) or mechanical pulping (Lee, Matsuoka & Sumimoto, 1990). Stilbenes (1*a*) and (2*a*) are model compounds representative of such stilbene structures. Acid-catalysed reactions of phenylcoumaran structures also give rise to stilbenes. Stilbene (2*a*) (m.p. 439 K, from ethyl acetate) is obtained on acid treatment of a model compound of the phenylcoumaran type [*trans*-2-(3,4-dimethoxyphenyl)-2,3-dihydro-3-hydroxymethyl-7-methoxybenzofuran] (Li, Lundquist & Stomberg, 1996). To ensure the steric assignments of stilbenes (1) and (2), we have examined the acetate derivative of (1*a*) [*i.e.* compound (1*b*)] by X-ray crystallography.



(1*a*) *R*=H (2*a*) *R*=H
(1*b*) *R*=$COCH_3$ (2*b*) *R*=$COCH_3$

Stilbene (1*b*) was obtained by decarboxylation of (5) (see reaction scheme). The decarboxylation reaction also leads to the formation of the isomeric stilbene (2*b*). The formation of this latter stilbene is unexpected, since the decarboxylation of acids of type (5) are reported to occur with retention of the configuration (*cf.* Battersby & Greenock, 1961). The starting material (5) was prepared by condensation of (3) with (4) in a reaction of the Perkin type (see reaction scheme). Substantial amounts of lactone (6) were obtained as a by-product.

The crystal structure determination demonstrates unambiguously that (1*b*) has the *Z* configuration. Fig. 1 gives a perspective view of (1*b*) with the atomic numbering. The angle between the aromatic ring planes is 55.1 (1)°. The torsion angles C2—C1—C7—C8 and C7—C8—C11—C16 are 36.7 (5) and 55.2 (5)°, respectively. Similar conformations are adopted by other (*Z*)-stilbene derivatives examined by X-ray crystallography, *e.g.* (*Z*)-2-nitrostilbene (Todres, Gridunova, Dyusengaliev & Struchkov, 1987), (*Z*)-5-methoxymethyl-3-[4-(phenylethenyl)phenyl]-2-oxazolidinone (Durant, Lefevre, Norberg & Evrard, 1982),



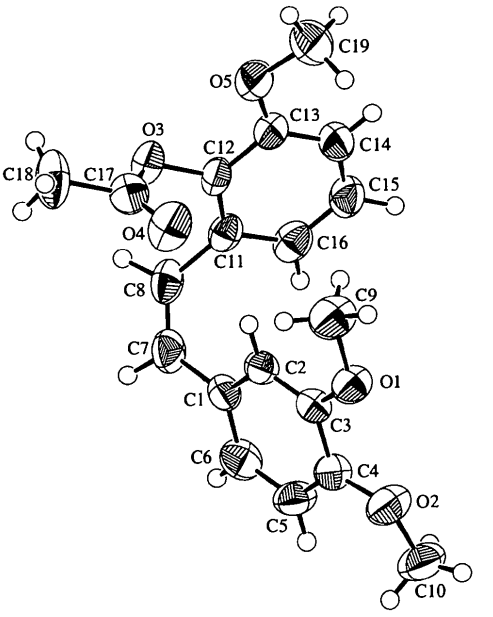


Fig. 1. A perspective drawing (*ORTEP*II; Johnson, 1976) of (1*b*) with displacement ellipsoids at the 50% level, showing the numbering of the non-H atoms. H atoms are shown as small spheres of arbitrary diameter.

combretastatin A-1 (Pettit, Singh, Niven, Hamel & Schmidt, 1987), (*Z*,*Z*)-1,4-bis(3,5-di-*tert*-butylstyryl)-benzene (Håkansson, Jagner, Sundahl & Wennerström, 1992) and (*Z*,*Z*)-1,2-distyrylbenzene (Böhm, Adam, Mauermann, Stein & Müllen, 1992). In (*Z*)-stilbene, the torsion angles corresponding to C2—C1—C7—C8 and C7—C8—C11—C16 have been determined to be *ca* 43° by electron diffraction methods in the gas phase (Traetteberg & Frantsen, 1975). The deviations from planarity can be explained by steric hindrance (interactions between the aromatic rings). In (*E*)-stilbenes, there is no steric interaction between the aromatic rings and such compounds are almost planar provided they are lacking substituents in the ring positions adjacent to the ethylenic group [*e.g.* (*E*)-stilbene (Ogawa, Sano, Yoshimura, Takeuchi & Toriumi, 1992) and (*E*)-4,4′-dimethoxystilbene (Theocharis, Jones & Rao, 1984)]. Disregarding some exceptions [*e.g.* the tetraacetate of chlorophorin (Krohn *et al.*, 1986) and (*E*)-2-acetoxy-3,3′,4′-trimethoxystilbene (2*b*) (Li, Lundquist & Stomberg, 1996)], (*E*)-stilbenes with substituents in the positions adjacent to the ethylenic group exhibit pronounced deviations from planarity (see *e.g.* Ogawa *et al.*, 1992).

The angles C7—C8—C11 [125.0 (3)°] and C8—C7—C1 [127.4 (3)°] in (1*b*) are comparatively large and the values deviate from normal ones; this is also true for the corresponding angles in other stilbenes (see the literature referred to above). The C and O atoms of the acetoxy group in (1*b*) are coplanar within 1σ. The plane thus defined forms an angle of 86.0 (1)° with the C11—C16 aromatic ring.

Experimental

(*E*)-3-(2-Acetoxy-3-methoxyphenyl)-2-(3,4-dimethoxyphenyl)-propenoic acid, (5), was prepared starting from 2-acetoxy-3-methoxybenzaldehyde (2.91 g) and (3,4-dimethoxyphenyl)-acetic acid (3.14 g) using a procedure analogous to that applied for the synthesis of (*E*)-2,3-bis(3,4-dimethoxyphenyl)propenoic acid (Walker, 1954). The crude product was dissolved in chloroform and the solution was extracted with aqueous $NaHCO_3$ (saturated solution). A crystalline precipitate was obtained on acidification (hydrochloric acid) of the extract. Recrystallization from acetone gave (5) (1.08 g) of m.p. 460–462 K [Gierer, Lenic, Norén & Szabo-Lin (1974) report m.p. 461–464 K]. The steric assignment of (5) could be ensured by NMR spectral comparisons with related compounds with established stereochemistry (Stomberg, Li & Lundquist, 1995, 1996). ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 293 K, TMS): δ 2.38 (3*H*, *s*; CH_3CO), 3.70 (3*H*, *s*; OCH_3), 3.81 (3*H*, *s*; OCH_3), 3.87 (3*H*, *s*; OCH_3), 6.38 (1*H*, *dd*, J = 1.4 and 8 Hz; H–Ar), 6.7–6.9 (5*H*, *m*; H–Ar), 7.87 (1*H*, *s*; vinyl H).

Evaporation of the solvent from the chloroform layer gave an oily residue. Crystals (1.47 g) with unsharp m.p. were obtained from ethanol. Recrystallization gave a product of m.p. 422–423 K. The compound was identified as the lactone (6) on the basis of ^{1}H NMR spectral examinations; compound (6) has been described by Gierer, Lenic *et al.* (1974). ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 293 K, TMS): δ 3.93 (3*H*, *s*; OCH_3), 3.95 (3*H*, *s*; OCH_3), 3.99 (3*H*, *s*; OCH_3), 6.9–7.4 (6*H*, *m*; H–Ar), 7.76 (1*H*, *s*; vinyl H).

The *Z* (1*b*) and *E* (2*b*) forms of 2-acetoxy-3,3′,4′-trimethoxy-stilbene were obtained on decarboxylation of (5) (0.50 g) using

the method applied by Battersby & Greenock (1961) for the decarboxylation of (*E*)-2,3-bis(3,4-dimethoxyphenyl)propenoic acid. The products are only slightly soluble in ether and the work-up procedure used by Battersby & Greenock (1961) was therefore modified in the respect that ether as well as chloroform was used in the extraction step. The crude product was chromatographed [40 g SiO_2 (Grace, Matrex LC 60 Å/35–70 μm); eluent, hexane-acetone (5:1)]. Stilbene (1*b*) (75 mg) was eluted before stilbene (2*b*). The fraction containing (2*b*) (80 mg) was contaminated with (2*a*). Crystallization of (1*b*) from ethyl acetate gave a product melting at 373–374 K [Gierer, Lenic *et al.* (1974) report m.p. 376–377 K]. ^{1}H NMR spectrum of (1*b*) (400 MHz, $CDCl_3$, 293 K, TMS): δ 2.29 (3*H*, *s*; CH_3CO), 3.56 (3*H*, *s*; OCH_3), 3.83 (3*H*, *s*; OCH_3), 3.84 (3*H*, *s*; OCH_3), 6.38 (1*H*, *d*, *J* = 11.9 Hz; vinyl H), 6.59 (1*H*, *d*, *J* = 11.9 Hz; vinyl H), 6.7–6.9 (5*H*, *m*; H–Ar), 7.02 (1*H*, *t*, *J* = 8 Hz; H–Ar). Acetylation of the fraction containing (2*a*) and (2*b*) [acetic anhydride/pyridine (1:1), 24 h] gave (2*b*) (m.p. 374–375 K). ^{1}H NMR spectrum of (2*b*) (400 MHz, $CDCl_3$, 293 K, TMS): δ 2.38 (3*H*, *s*; CH_3CO), 3.85 (3*H*, *s*; OCH_3), 3.91 (3*H*, *s*; OCH_3), 3.94 (3*H*, *s*; OCH_3), 6.96 (1*H*, *d*, *J* = 16.4 Hz; vinyl H), 7.05 (1*H*, *d*, *J* = 16.4 Hz; vinyl H), 6.8–7.3 (6*H*, *m*; H–Ar).

Crystal data

$C_{19}H_{20}O_5$
M_r = 328.35
Orthorhombic
Pbca
a = 17.5555 (11) Å
b = 7.3717 (7) Å
c = 26.736 (2) Å
V = 3460.0 (5) Å^3
Z = 8
D_x = 1.261 Mg m^{-3}
D_m not measured

Mo *Kα* radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 12.0–18.0°
μ = 0.091 mm^{-1}
T = 293 (2) K
Fragment
0.5 × 0.5 × 0.4 mm
Colourless

Data collection

CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
3504 measured reflections
3504 independent reflections
1476 observed reflections [$I > 2\sigma(I)$]

θ_{max} = 26.29°
h = 0 → 21
k = −9 → 0
l = −33 → 0
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.0474
$wR(F^2)$ = 0.1629
S = 1.000
3495 reflections
222 parameters
H atoms riding
$w = 1/[\sigma^2(F_o^2) + (0.0330P)^2 + 2.1400P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = −0.034

$\Delta\rho_{max}$ = 0.177 e Å^{-3}
$\Delta\rho_{min}$ = −0.193 e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.0035 (4)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

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

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

	x	*y*	*z*	U_{eq}
C1	0.1288 (2)	0.1592 (4)	0.34620 (12)	0.0491 (8)
C2	0.0876 (2)	0.1893 (4)	0.39026 (11)	0.0478 (8)
C3	0.1201 (2)	0.1718 (4)	0.43654 (11)	0.0463 (8)
C4	0.1978 (2)	0.1254 (5)	0.44030 (12)	0.0526 (9)
C5	0.2374 (2)	0.0870 (5)	0.39746 (13)	0.0637 (10)
C6	0.2033 (2)	0.1025 (5)	0.35109 (13)	0.0625 (10)
C7	0.0939 (2)	0.1814 (5)	0.29683 (12)	0.0614 (10)
C8	0.0431 (2)	0.3052 (5)	0.28306 (12)	0.0597 (10)
C9	0.0044 (2)	0.2445 (6)	0.47818 (13)	0.0767 (12)
C10	0.3081 (2)	0.1220 (6)	0.49222 (14)	0.0809 (13)
C11	0.0173 (2)	0.4569 (5)	0.31432 (11)	0.0488 (8)
C12	−0.0590 (2)	0.4818 (4)	0.32500 (11)	0.0471 (8)
C13	−0.0849 (2)	0.6191 (5)	0.35653 (12)	0.0555 (9)
C14	−0.0327 (2)	0.7388 (5)	0.37620 (13)	0.0647 (10)
C15	0.0438 (2)	0.7189 (5)	0.36522 (13)	0.0638 (10)
C16	0.0685 (2)	0.5809 (5)	0.33542 (12)	0.0597 (10)
C17	−0.1331 (2)	0.2152 (5)	0.32642 (14)	0.0563 (9)
C18	−0.1837 (2)	0.1008 (6)	0.29452 (14)	0.0818 (13)
C19	−0.1886 (2)	0.7378 (6)	0.40424 (14)	0.0831 (13)
O1	0.08330 (12)	0.1988 (3)	0.48083 (7)	0.0585 (6)
O2	0.22694 (12)	0.1193 (4)	0.48763 (8)	0.0706 (8)
O3	−0.11235 (12)	0.3677 (3)	0.30169 (8)	0.0572 (6)
O4	−0.11212 (14)	0.1820 (4)	0.36784 (10)	0.0765 (8)
O5	−0.16158 (14)	0.6225 (4)	0.36505 (9)	0.0761 (8)

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

C1—C6	1.379 (4)	C11—C12	1.382 (4)
C1—C2	1.400 (4)	C11—C16	1.401 (4)
C1—C7	1.464 (4)	C12—C13	1.393 (4)
C2—C3	1.368 (4)	C12—O3	1.404 (3)
C3—O1	1.363 (3)	C13—O5	1.366 (4)
C3—C4	1.410 (4)	C13—C14	1.376 (4)
C4—O2	1.366 (4)	C14—C15	1.383 (5)
C4—C5	1.370 (4)	C15—C16	1.363 (5)
C5—C6	1.382 (4)	C17—O4	1.192 (4)
C7—C8	1.328 (4)	C17—O3	1.354 (4)
C8—C11	1.468 (5)	C17—C18	1.493 (5)
C9—O1	1.427 (4)	C19—O5	1.430 (4)
C10—O2	1.430 (4)		
C6—C1—C7	121.1 (3)	C11—C12—O3	118.3 (3)
C2—C1—C7	121.6 (3)	C13—C12—O3	119.1 (3)
O1—C3—C2	125.1 (3)	O5—C13—C14	125.5 (3)
O1—C3—C4	115.6 (3)	O5—C13—C12	115.8 (3)
O2—C4—C5	125.3 (3)	O4—C17—O3	122.7 (3)
O2—C4—C3	115.9 (3)	O4—C17—C18	126.8 (4)
C8—C7—C1	127.4 (3)	C3—O1—C9	116.8 (2)
C7—C8—C11	125.0 (3)	C4—O2—C10	116.9 (3)
C12—C11—C8	121.2 (3)	C17—O3—C12	117.4 (2)
C16—C11—C8	121.8 (3)	C13—O5—C19	117.4 (3)
C6—C1—C7—C8	−145.1 (4)	C4—C3—O1—C9	−179.6 (3)
C2—C1—C7—C8	36.7 (5)	C5—C4—O2—C10	17.9 (5)
C1—C7—C8—C11	6.2 (6)	O4—C17—O3—C12	5.3 (5)
C7—C8—C11—C12	−123.6 (4)	C18—C17—O3—C12	−174.4 (3)
C7—C8—C11—C16	55.2 (5)	C11—C12—O3—C17	92.4 (3)
C8—C11—C12—O3	−5.5 (4)	C14—C13—O5—C19	−11.9 (5)
O3—C12—C13—O5	4.7 (4)		

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1992). Cell refinement: *CAD-4 EXPRESS*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1985). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *TEXSAN*. Software used to prepare material for publication: *SHELXL*93.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KA1212). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Adler, E., Marton, J. & Falkehag, I. (1964). *Acta Chem. Scand.* **18**, 1311–1312.

Battersby, A. R. & Greenock, I. A. (1961). *J. Chem. Soc.* pp. 2592–2593.

Böhm, A., Adam, M., Mauermann, H., Stein, S. & Müllen, K. (1992). *Tetrahedron Lett.* **33**, 2795–2798.

Durant, F., Lefevre, F., Norberg, B. & Evrard, G. (1982). *Cryst. Struct. Commun.* **11**, 983–990.

Enraf–Nonius (1992). *CAD-4 EXPRESS*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.

Gierer, J., Lenic, J., Norén, I. & Szabo-Lin, I. (1974). *Acta Chem. Scand. Ser. B*, **28**, 717–729.

Gierer, J., Pettersson, I. & Szabo-Lin, I. (1974). *Acta Chem. Scand. Ser. B*, **28**, 1129–1135.

Håkansson, M., Jagner, S., Sundahl, M. & Wennerström, O. (1992). *Acta Chem. Scand.* **46**, 1160–1165.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Krohn, K., Müller, H., Adiwidjaja, G., Jarchow, O. H., Schmalle, H. W., Hausen, B. M. & Schulz, K.-H. (1986). *Z. Kristallogr.* **174**, 283–290.

Lee, D.-Y., Matsuoka, M. & Sumimoto, M. (1990). *Holzforschung*, **44**, 415–418.

Li, S., Lundquist, K. & Stomberg, R. (1996). Unpublished data.

Molecular Structure Corporation (1985). *TEXSAN. TEXRAY Structure Analysis Package*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Ogawa, K., Sano, T., Yoshimura, S., Takeuchi, Y. & Toriumi, K. (1992). *J. Am. Chem. Soc.* **114**, 1041–1051.

Pettit, G. R., Singh, S. B., Niven, M. L., Hamel, E. & Schmidt, J. M. (1987). *J. Nat. Prod.* **50**, 119–131.

Sheldrick, G. M. (1985). *SHELXS86. Program for the Solution of Crystal Structures*. University of Göttingen, Germany.

Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Stomberg, R., Li, S. & Lundquist, K. (1995). *Acta Cryst.* C**51**, 2698–2700.

Stomberg, R., Li, S. & Lundquist, K. (1996). *Z. Kristallogr.* **211**, 585–586.

Theocharis, C. R., Jones, W. & Rao, C. N. R. (1984). *J. Chem. Soc. Chem. Commun.* pp. 1291–1293.

Todres, Z. V., Gridunova, G. V., Dyusengaliev, K. I. & Struchkov, Yu. T. (1987). *Zh. Org. Khim.* **23**, 1805–1807.

Traetteberg, M. & Frantsen, E. B. (1975). *J. Mol. Struct.* **26**, 69–76.

Walker, G. N. (1954). *J. Am. Chem. Soc.* **76**, 3999–4003.

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Quitenidinium Ethyl Ester Ethyl Sulfate

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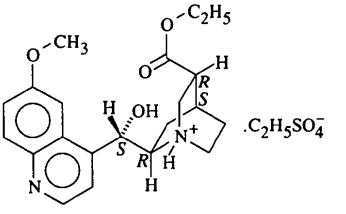
Abstract

The crystal structure of quitenidinium ethyl ester ethyl sulfate, $C_{21}H_{27}N_2O_4^+.C_2H_5SO_4^-$ has been determined. The conformation of the cation is open in contrast to the closed conformation of the non-protonated quitenine ethyl ester. The molecules are linked by intermolecular O—H···N hydrogen bonds into chains along the *b* axis. A bifurcated hydrogen bond is present between the protonated quinuclidine N and two O atoms belonging to the ethyl sulfate anion.

Comment

The title compound, $QtdEE^+.ES^-$ (QtdEE = quitenidinium ethyl ester; ES = ethyl sulfate), (I), is a salt which consists of an esterified quitenidine cation and an ethyl sulfate anion. Quitenidine is a derivative of the anti-arrhythmic and antimalarial alkaloid, quinidine, in which the vinyl group at C3 of the quinuclidine moiety is oxidized to carboxyl. The positive charge of $QtdEE^+$ is due to the protonated N atom, N1, of quinuclidine.



(I)

The aim of the X-ray structure analysis of $QtdEE^+.ES^-$ is to determine the conformation of the cation and the mode of its interaction with the anion since these two properties are important in recognition of quinidine and its derivatives by their biological receptors. It is also interesting to compare the structures of this protonated quitenidine ester and its non-protonated quitenine analogue (QtEE) reported recently (Lewinski, Nitek, Oleksyn & Stec, 1995) in order to check the ef-