Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
698 measured reflections
671 independent reflections
528 observed reflections [$I \geq 2.5\sigma(I)$]
$R_{\rm int} = 0.011$
$\theta_{\rm max} = 28°$
$h = 0 \rightarrow 17$
$k = 0 \rightarrow 8$
$l = -7 \rightarrow 7$
3 standard reflections
frequency: 60 min
intensity variation: 0.1%

Refinement

Refinement on F
$R = 0.049$
$wR = 0.059$
$S = 2.79$
528 reflections
60 parameters
All H-atom parameters refined
$w = 1/\sigma^2(F_o)$
$(\Delta/\sigma)_{\rm max} < 0.01$
$\Delta\rho_{\rm max} = 0.20$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.36$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

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

	x	y	z	$U_{\rm eq}$
O1	0.7286 (1)	0	−0.0582 (3)	0.055 (1)
O2	0.7827 (1)	0	0.3044 (2)	0.048 (1)
C1	0.9018 (1)	0	0.0334 (3)	0.038 (1)
C2	0.9769 (1)	0.1710 (3)	0.1187 (2)	0.045 (1)
C3	0.9491 (1)	0	−0.2030 (4)	0.044 (1)
C4	0.7955 (1)	0	0.0807 (3)	0.037 (1)
C5	0.6830 (2)	0	0.3772 (4)	0.058 (1)

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

O1—C4	1.199 (2)	C1—C3	1.556 (3)
O2—C4	1.336 (2)	C1—C4	1.481 (3)
O2—C5	1.436 (3)	C2—C2″	1.555 (2)
C1—C2	1.570 (2)	C2—C3″	1.559 (2)
O1···C3	3.143 (3)	C4···C3″	3.517 (3)
O1···C5	2.663 (3)	O2···C2	3.095 (2)
O1—C4—O2	123.5 (2)	C2—C1—C4	124.5 (1)
O1—C4—C1	126.2 (2)	C2—C1—C2′	89.0 (1)
O2—C4—C1	110.4 (2)	C2—C2″—C3	90.6 (1)
C1—C2—C2″	89.5 (1)	C2—C3″—C2′	89.8 (1)
C1—C2—C3″	90.6 (1)	C3—C1—C4	127.3 (2)
C1—C3—C2″	89.8 (1)	C4—O2—C5	116.9 (2)
C2—C1—C3	90.1 (1)		

The selection of the space group *C2/m* is based on statistics of the reflection intensities. Structure solution was carried out using *MULTAN*11/82 (Main *et al.*, 1982).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: SE1048). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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(*Z*)-2-(2-Methoxyphenoxy)-3-(4-methoxyphenyl)propenoic Acid

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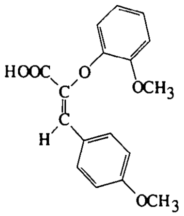
Abstract

The structure of (*Z*)-2-(2-methoxyphenoxy)-3-(4-methoxyphenyl)propenoic acid, $C_{17}H_{16}O_5$, was

elucidated by X-ray crystallography. Stereoselective hydroboration/oxidation of this compound gave *erythro*-2-(2-methoxyphenoxy)-3-(4-methoxyphenyl)-1,3-propanediol. The outcome of the reaction confirms an earlier steric assignment of this latter compound.

Comment

α-Aryloxycinnamic acids are intermediates in stereoselective syntheses of lignin model compounds of the arylglycerol β-aryl ether type (Ahvonen, Brunow, Kristersson & Lundquist, 1983) and lignin-related enol ethers (Brunow & Lundquist, 1984). The X-ray work presented in this paper establishes the structure and stereochemistry of such an intermediate, namely (*Z*)-2-(2-methoxyphenoxy)-3-(4-methoxyphenyl)propenoic acid, (I).



(I)

A perspective view of a molecule of the title compound is shown in Fig. 1. The molecules in the crystals are held together in pairs by strong hydrogen bonds between the carboxyl groups (Table 2). The angles C(6)—C(1)—C(8) [125.0 (2)°] and C(1)—C(8)—C(9) [129.9 (2)°] have values that deviate considerably from 'normal' ones (*i.e.* ~120°). The deviations lead to an increase in the distance between the atoms H(C6) and O(2). This distance was determined to be 2.35 (2) Å, whereas with 'normal' angles it would have been about 1.8 Å. The increased separation of H(C6) and O(2) reduces the steric interaction between these two atoms. Interestingly, semi-empirical quantum-mechanical calculations (Norinder, 1993) using the AM1 method (Stewart, 1990) gave values for the topical angles [C(6)—C(1)—C(8) 122.8, C(1)—C(8)—C(9) 128.1°] that are close to those determined by X-ray crystallography. Analogous deviations from normal bond angles were found in the related compound (*Z*)-2-(2,6-dimethoxyphenoxy)-3-(3,4-dimethoxyphenyl)propenoic acid (Lundquist, Stomberg & von Unge, 1987).

The eight atoms between the two aromatic rings are located near the plane they define (maximum deviation 15σ) and this plane forms an angle of 8.8 (2)° with the C(1)–C(6) aromatic ring. The benzylic C atom [C(8)] is twisted 0.086 (3) Å from the C(1)–C(6) ring plane, while the atom connecting the other aromatic ring [C(11)–C(16)] to the rest of the molecule [O(2)] is situated very near the C(11)–C(16) ring plane [deviation 0.011 (3) Å]. The angle between the aromatic ring planes is 81.6 (3)°. The short non-bonding intermolecular contact distances of 3.284 (3) [O(4)···O(4)($1-x$, $1-y$, $2-z$)], 2.45 (3) [C(10)···H(O3)($1-x$, $1-y$, $2-z$)] and 2.22 (6) Å [H(O3)···H(O3)($1-x$, $1-y$, $2-z$)] are consequences of the hydrogen-bond interaction.

Treatment of a small amount of (*Z*)-2-(2-methoxyphenoxy)-3-(4-methoxyphenyl)propenoic acid (1 mmol) with $BH_3.S(CH_3)_2/H_2O_2$, OH^-, according to a method previously used for the reduction and hydration of α-aryloxycinnamic acids (Ahvonen, Brunow, Kristersson & Lundquist, 1983) gave the lignin model compound *erythro*-2-(2-methoxyphenoxy)-3-(4-methoxyphenyl)-1,3-propanediol in 40–50% yield (from ^{1}H NMR spectra of the acetylated reaction product), trace amounts of the *threo*-isomer were possibly present in the reaction mixture. The *erythro* and *threo* forms of 2-(2-methoxyphenoxy)-3-(4-methoxyphenyl)-1,3-propanediol were assigned in a previous paper on the basis of studies of the stability of their borate complexes and ^{1}H NMR spectral comparisons (Ibrahim & Lundquist, 1994). The hydroboration/oxidation experiment with (*Z*)-2-(2-methoxyphenoxy)-3-(4-methoxyphenyl)propenoic acid confirms the assignments since the stereoselective hydroboration/oxidation reaction of this compound should give the

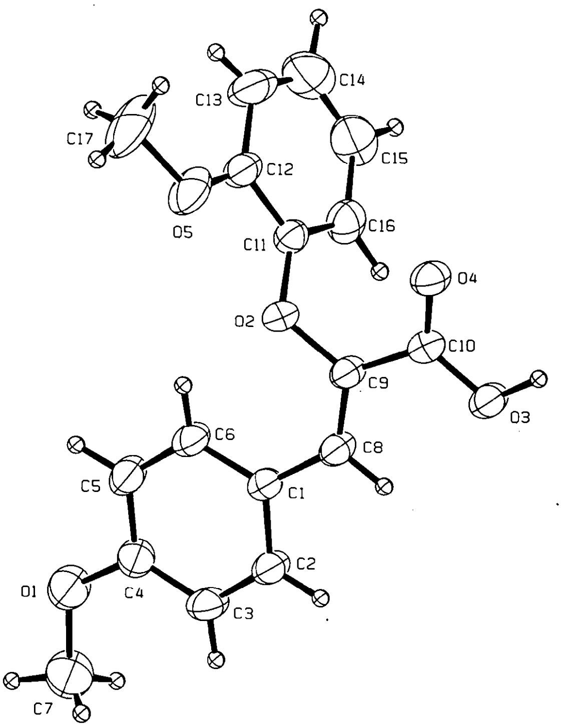


Fig. 1. A perspective drawing (*ORTEP*; Johnson, 1976) of the title compound with displacement ellipsoids at the 30% probability level.

erythro form of 2-(2-methoxyphenoxy)-3-(4-methoxyphenyl)-1,3-propanediol [*cf.* the analogous hydroboration/oxidation reactions of related α-aryloxycinnamic acids reported earlier (Ahvonen, Brunow, Kristersson & Lundquist, 1983; Brunow & Lundquist, 1984; Lundquist, Stomberg & von Unge, 1987; Brunow, Sipilä, Lundquist & von Unge, 1988)].

Experimental

The title compound, (*Z*)-2-(2-methoxyphenoxy)-3-(4-methoxyphenyl)propenoic acid, was prepared from anisaldehyde (5.2 g, 38 mmol) and methyl (2-methoxyphenoxy)ethanoate (7.5 g, 38 mmol) according to a procedure previously developed for the synthesis of (*Z*)-3-(3,4-dimethoxyphenyl)-2-(2-methoxyphenoxy)propenoic acid (Berndtsson & Lundquist, 1977). A product (3.3 g) melting at 454–456 K was obtained from acetone. ^{1}H NMR (CDCl$_3$, 292 K): δ 3.80 (3H, *s*, OCH$_3$), 3.96 (3H, *s*, OCH$_3$), 7.45 (1H, *s*, vinyl H) and 6.7–7.8 p.p.m. (8H, *m*, aromatic H).

Crystal data

$C_{17}H_{16}O_5$
$M_r = 300.31$
Triclinic
$P\bar{1}$
$a = 10.113\ (2)$ Å
$b = 10.546\ (2)$ Å
$c = 8.618\ (1)$ Å
$\alpha = 105.64\ (2)°$
$\beta = 102.10\ (2)°$
$\gamma = 113.63\ (2)°$
$V = 756.5\ (3)$ Å^3
$Z = 2$
$D_x = 1.318$ Mg m^{-3}

Cu $K\alpha$ radiation
$\lambda = 1.54178$ Å
Cell parameters from 20 reflections
$\theta = 21.6–24.7°$
$\mu = 0.77$ mm^{-1}
$T = 296$ K
Prism
$0.66 \times 0.21 \times 0.18$ mm
Colourless

Data collection

Syntex $P2_1$ diffractometer
ω–2θ scans
Absorption correction: none
2401 measured reflections
2253 independent reflections
1802 observed reflections [$I > 3\sigma(I)$]
$R_{\rm int} = 0.024$

$\theta_{\rm max} = 60.0°$
$h = 0 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -10 \rightarrow 10$
3 standard reflections monitored every 150 reflections intensity variation: -2.3, -1.3 and -6.8%

Refinement

Refinement on F
$R = 0.042$
$wR = 0.053$
$S = 2.37$
1692 reflections
263 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o) + 0.03(F_o)^2]$

$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.25$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.18$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

$$B_{\rm eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
C(1)	0.3714 (2)	0.2439 (2)	0.2784 (3)	4.00 (7)
C(2)	0.2291 (3)	0.1849 (3)	0.1515 (3)	4.76 (8)
C(3)	0.2019 (3)	0.1157 (3)	−0.0206 (3)	5.3 (1)
C(4)	0.3183 (3)	0.1059 (3)	−0.0699 (3)	5.02 (8)
C(5)	0.4617 (3)	0.1644 (3)	0.0525 (3)	5.7 (1)
C(6)	0.4874 (3)	0.2321 (3)	0.2235 (3)	5.16 (9)
C(7)	0.1651 (5)	−0.0085 (6)	−0.3708 (5)	9.2 (2)
C(8)	0.3868 (3)	0.3062 (3)	0.4589 (3)	4.56 (8)
C(9)	0.5102 (2)	0.3696 (3)	0.6040 (3)	4.42 (8)
C(10)	0.5051 (3)	0.4253 (2)	0.7769 (3)	4.27 (8)
C(11)	0.7314 (2)	0.3408 (3)	0.6759 (3)	4.22 (7)
C(12)	0.8905 (3)	0.4153 (3)	0.7308 (3)	5.36 (9)
C(13)	0.9705 (5)	0.3547 (7)	0.8109 (4)	8.3 (2)
C(14)	0.8920 (8)	0.2248 (7)	0.8324 (6)	9.9 (2)
C(15)	0.7380 (6)	0.1518 (5)	0.7757 (5)	8.3 (2)
C(16)	0.6552 (4)	0.2076 (3)	0.6966 (4)	5.9 (1)
C(17)	1.1185 (4)	0.6140 (7)	0.7380 (8)	11.6 (2)
O(1)	0.3047 (2)	0.0398 (2)	−0.2371 (2)	7.27 (8)
O(2)	0.6561 (2)	0.4038 (2)	0.5987 (2)	4.65 (5)
O(3)	0.3691 (2)	0.3968 (2)	0.7814 (2)	5.45 (6)
O(4)	0.6242 (2)	0.4933 (2)	0.9065 (2)	5.00 (6)
O(5)	0.9545 (2)	0.5438 (2)	0.7033 (3)	7.44 (8)
H(O3)	0.380 (3)	0.448 (4)	0.908 (4)	9.4 (9)

Table 2. *Bond lengths* (Å), *bond angles* (°), *torsion angles* (°) *and hydrogen-bonding geometry* (Å, °)

C(1)—C(8)	1.463 (3)	C(10)—O(3)	1.297 (3)
C(4)—O(1)	1.370 (3)	C(10)—O(4)	1.234 (3)
C(7)—O(1)	1.417 (4)	C(11)—O(2)	1.377 (3)
C(8)—C(9)	1.339 (3)	C(12)—O(5)	1.359 (3)
C(9)—C(10)	1.467 (3)	C(17)—O(5)	1.441 (4)
C(9)—O(2)	1.386 (3)		

C(2)—C(1)—C(8)	118.2 (2)	C(9)—C(10)—O(4)	120.8 (2)
C(6)—C(1)—C(8)	125.0 (2)	O(3)—C(10)—O(4)	123.9 (2)
C(3)—C(4)—O(1)	124.8 (2)	C(12)—C(11)—O(2)	116.6 (2)
C(5)—C(4)—O(1)	115.3 (2)	C(16)—C(11)—O(2)	123.4 (2)
C(1)—C(8)—C(9)	129.9 (2)	C(11)—C(12)—O(5)	115.7 (2)
C(8)—C(9)—C(10)	123.0 (2)	C(13)—C(12)—O(5)	126.3 (3)
C(8)—C(9)—O(2)	121.2 (2)	C(4)—O(1)—C(7)	118.1 (3)
C(10)—C(9)—O(2)	115.3 (2)	C(9)—O(2)—C(11)	117.0 (2)
C(9)—C(10)—O(3)	115.3 (2)	C(12)—O(5)—C(17)	117.1 (4)

C(1)—C(8)—C(9)—C(10)	−179.2 (2)
C(1)—C(8)—C(9)—O(2)	9.0 (4)
C(2)—C(1)—C(8)—C(9)	−179.7 (3)
C(2)—C(1)—C(8)—H(C8)	0 (1)
C(2)—C(3)—C(4)—O(1)	180.0 (2)
C(3)—C(4)—O(1)—C(7)	6.9 (5)
C(8)—C(9)—C(10)—O(3)	6.0 (3)
C(8)—C(9)—C(10)—O(4)	−174.4 (2)
C(8)—C(9)—O(2)—C(11)	−122.9 (2)
C(9)—C(10)—O(3)—H(O3)	−175 (2)
C(9)—O(2)—C(11)—C(12)	−155.5 (2)
C(10)—C(9)—O(2)—C(11)	64.8 (3)
C(11)—C(12)—O(5)—C(17)	−172.1 (3)
C(13)—C(12)—O(5)—C(17)	9.1 (5)
O(2)—C(9)—C(8)—H(C8)	−171 (1)
O(2)—C(9)—C(10)—O(3)	178.2 (2)
O(2)—C(9)—C(10)—O(4)	−2.2 (3)
O(4)—C(10)—O(3)—H(O3)	5 (2)

D—H···*A*	H···*A*	*D*···*A*	*D*—H···*A*
O(3)—H(O3)···O(4$^{\rm i}$)	1.57 (4)	2.600 (3)	172 (3)

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

Symmetry and approximate cell dimensions were derived from rotation and Weissenberg photographs (Cu $K\alpha$ radiation). The *TEXSAN* crystallographic software package (Molecular Structure Corporation, 1985) [including *SHELXS*86 (Sheldrick, 1985)] was used for solving and refining the structure.

We thank A. Johansson MSc for preliminary synthesis of the title compound.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry, including H-atom geometry, have been deposited with the IUCr (Reference: AB1137). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Two Dimethylmorpholinium Bromides

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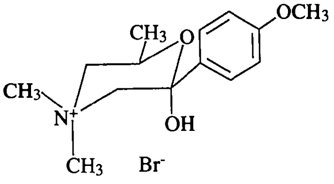
Abstract

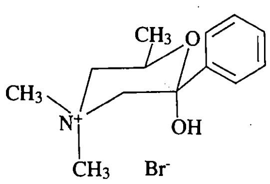
In the title compounds 2-hydroxy-2-(4-methoxyphenyl)-4,4,6-trimethylmorpholinium bromide, $C_{14}H_{22}NO_3^+.Br^-$, (1), and 2-hydroxy-4,4,6-trimethyl-2-phenylmorpholinium bromide hydrate, $C_{13}H_{20}NO_2^+.Br^-.xH_2O$, (2), the morpholinium rings adopt a chair conformation with the magnitudes of the endocyclic torsion angles in (1) and (2) in the ranges 50.5 (7)–60.1 (7) and 49.4 (4)–58.3 (4)°, respectively. The hydroxyl group is in the axial position of the morpholinium ring in both structures with C—OH bond distances of 1.410 (9) and 1.409 (4) Å. In (2), the hydroxy H atom points towards a Br ion [O···Br 3.246 (3), H···Br 2.55 (3) Å, O—H···Br 172 (3)°]. The OH···Br interaction in (1) is longer and nonlinear [O···Br 3.427 (5) Å, O—H···Br 123 (8)°].

Comment

As part of a larger study of structural changes in reactions involving tetrahedral intermediates and substituent effects in 2-substituted 2-hydroxy-4,4-dimethylmorpholinium bromides (Lee *et al.*, 1992), the syntheses of some morpholinium bromides (Garcia-Guajardo, Fronczek & Gandour, 1986; Altbach *et al.*, 1988; Garcia, Fronczek & Gandour, 1992*a*, 1993*a*) were performed. 2-Hydroxy-2-(4-methoxyphenyl)-4,4-dimethyl-6-methylmorpholinium bromide (1) was prepared by condensing 4-methoxy-2′-bromoacetophenone with 2-hydroxy-*N*,*N*-dimethylpropanol amine following the procedure described by Garcia (1986). Similarly, 2-hydroxy-4,4-dimethyl-6-methyl-2-phenylmorpholinium bromide hydrate (2) was prepared by condensing 2′-bromoacetophenone with 2-hydroxy-*N*,*N*-dimethylpropanol amine. Crystals of (1) (m.p. 443–445 K) and (2) (m.p. 480–482 K) were grown by slow cooling of methanol.



(1)



(2)

The average values of the O—CH3 and C(aromatic)—O distances and the C(aromatic)—O—CH3 angles in (1) [1.42 (1) and 1.372 (8) Å, 119.0 (6)°, respectively] are in agreement with those determined by X-ray crystallography by Nyburg & Faerman (1986) (1.425, 1.371 Å; 117.7°). Structural data for the title compounds are also in agreement with those for 2-(4-cyanophenyl)-2-hydroxy-4,4-dimethylmorpholinium bromide (Altbach *et al.*, 1988), 2-hydroxy-4,4-dimethyl-2-(4-tolyl)morpholinium bromide (Garcia, Fronczek & Gandour, 1992*a*), 2-hydroxy-2-(2-methylphenyl)-4,4-dimethylmorpholinium bromide (Garcia, Fronczek &

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