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(*Z*)-2,3-Bis(3,4-dimethoxyphenyl)-2-propen-1-ol

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.107
Data-to-parameter ratio = 12.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the crystal structure of the title compound, $C_{19}H_{22}O_5$, intermolecular hydrogen bonding gives rise to centrosymmetric dimers. The conformations of the title compound and its benzene solvate are compared.

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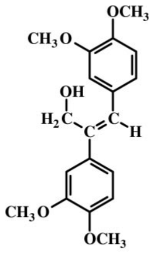
Comment

A series of diarylpropenols are present in reaction mixtures obtained on brief acid treatment of the lignin model 1,2-bis(3,4-dimethoxyphenyl)-1,3-propanediol or the *E* form of the diarylpropenols (Li *et al.*, 1997): (*Z*)-2,3-bis(3,4-dimethoxyphenyl)-2-propen-1-ol, (I), (*E*)-2,3-bis(3,4-dimethoxyphenyl)-2-propen-1-ol and 1,2-bis(3,4-dimethoxyphenyl)-2-propen-1-ol. Interestingly, Axenrod *et al.* (1965) obtained an analogous mixture of diphenylpropenols on acid treatment of (*E*)-2,3-diphenyl-2-propen-1-ol (or its isomers). Crystal structure determinations of a benzene solvate of (I) (Stomberg *et al.*, 1995) and (*E*)-2,3-bis(3,4-dimethoxyphenyl)-2-propen-1-ol (Stomberg *et al.*, 1994) provide proof of their stereochemical assignments. In connection with photophysical studies of diarylpropenols, the question arose as to whether the conformations of these compounds are similar in the crystal structures and in solution. We thought that a comparison of the conformations of (I) and its benzene solvate in the solid state could be of interest in this context. The crystal structure of (I) is described in this paper.



(I)

A perspective drawing of (I) and the atomic numbering are shown in Fig. 1. In the crystal structure, there are intermolecular bifurcated hydrogen bonds of the O—H···O type and a weak intramolecular hydrogen bond of the C—H···O type (Table 1). The intermolecular hydrogen bonds form centrosymmetric dimers (Fig. 2). On the first-level graph-set (Bernstein *et al.*, 1995; Grell *et al.*, 1999), the hydrogen bonds are classified as *S*(7) for the weak intramolecular hydrogen bond [*c*], while the hydrogen bonds [*a*] and [*b*] are classified as rings $R_2^2(16)$ and $R_2^2(18)$, respectively. On the second-level graph-set, rings $R_2^2(17)$ and $R_2^1(5)$ are formed by hydrogen bonds [*a*] and [*b*]. The assignment of graph-set descriptors was performed using *PLUTO*, as described by Motherwell *et al.* (1999).

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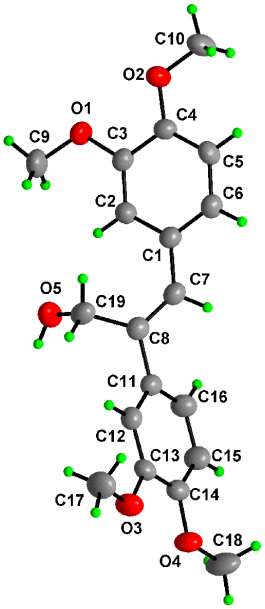

Figure 1
A perspective drawing of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

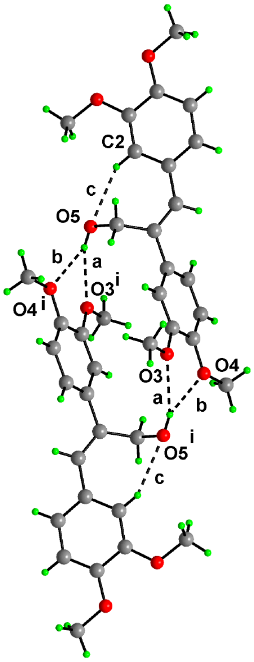

Figure 2
The hydrogen-bonding pattern of (I). A centrosymmetric dimer is formed [symmetry code: (i) $1-x, -y, 1-z$]. The hydrogen-bond notations are as given in Table 1.

The ethylenic C atoms and the atoms attached to them are almost coplanar in the crystal structures of (I) [r.m.s. deviation 0.019 Å and maximum deviation 0.025 (1) Å for atoms C1 and C11] and the benzene solvate of (I) [r.m.s. deviation 0.007 Å and maximum deviation 0.02 (3) Å for atom H7]. The aromatic rings are differently oriented in the two crystal structures: this is evident from the location of the methoxy groups attached to C3 and C13 [Table 2; Fig. 1 and the corresponding drawing in Stomberg *et al.* (1995)]. Nevertheless, the aromatic ring planes deviate from the ethylenic group plane in a similar manner in (I) and the benzene solvate of (I) (Table 2); the angle between the aromatic ring planes is 75.61 (6)° in (I) and 84.7° in its solvate. The overlap of π-orbitals is about the same in both crystal structures. Therefore, it seems reasonable to assume that the overlap of π-orbitals in solutions of (I) resembles the one adopted in the crystal structures.

Experimental

The synthesis of (I) (m.p. 403–404 K) has been described by Li *et al.* (1997).

Crystal data

$C_{19}H_{22}O_5$
$M_r = 330.37$
Triclinic, $P\overline{1}$
$a = 10.097$ (2) Å
$b = 10.358$ (2) Å
$c = 8.665$ (2) Å
$\alpha = 103.08$ (2)°
$\beta = 101.93$ (2)°
$\gamma = 78.10$ (2)°
$V = 851.5$ (3) Å^3
$Z = 2$
$D_x = 1.288$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 7.0$–$22.9°$
$\mu = 0.09$ mm^{-1}
$T = 295$ (2) K
Prism, colourless
0.34 × 0.23 × 0.18 mm

Data collection

Rigaku AFC-6 diffractometer
2θ–ω scans
Absorption correction: none
3180 measured reflections
2993 independent reflections
1665 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\rm max} = 25.0°$
$h = 0 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -10 \rightarrow 10$
3 standard reflections every 150 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.107$
$S = 1.00$
2993 reflections
245 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.1258P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.16$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.15$ e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.013 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5A···O3$^{\rm i}$ [*a*]	0.82	2.46	3.226 (2)	156
O5—H5A···O4$^{\rm i}$ [*b*]	0.82	2.28	2.940 (2)	138
C2—H2···O5 [*c*]	0.93	2.48	3.277 (3)	144

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

Table 2
Selected torsion angles (°) in (I) and the benzene solvate of (I).

Torsion angle	compound (I)	benzene solvate of (I)
C2—C1—C7—C8	−35.3 (3)	141.1 (3)
C1—C7—C8—C11	177.1 (2)	−179.2 (3)
C1—C7—C8—C19	−1.5 (4)	−0.7 (5)
C7—C8—C19—O5	92.6 (3)	88.0 (3)
C12—C11—C8—C7	140.3 (2)	−45.3 (4)

H atoms were refined isotropically and were constrained to an ideal geometry, using an appropriate riding model. For the hydroxyl group, the O—H distance (0.82 Å) and C—O—H angle (109.5°) were kept fixed, while the torsion angle was allowed to refine, with the starting position based on the circular Fourier synthesis. For methyl groups, the C—H distances (0.96 Å) and C—C—H angles (109.5°) were kept fixed, while the torsion angles were allowed to refine, with the starting position based on a threefold averaged circular Fourier synthesis. For aromatic H atoms, the C—H distance was kept fixed at 0.93 Å and for the secondary H atoms, the C—H distance was kept fixed at 0.97 Å. $U_{\rm iso}$(H) values were not restrained and were refined freely.

Data collection: *TEXSAN-TEXRAY* (Molecular Structure Corporation, 1985); cell refinement: *TEXSAN-TEXRAY*; data reduction: *TEXSAN-TEXRAY*; program(s) used to solve structure: *MITHRIL* (Gilmore, 1984); program(s) used to refine structure: *SHELXTL* (Bruker, 2001); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *SHELXTL*.

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