of Firmenich (Switzerland) for the crystals of compound (2). We thank Professor Bürgi for provision of computer facilities to prepare the figures.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: SH1094). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Carpenter, M. S., Easter, W. M. Jr & Wood, T. F. (1957). US Patent 2 800 511.

De Ridder, D. J. A. (1992). PhD thesis, pp. 137–162. Univ. of Amsterdam, The Netherlands.

De Ridder, D. J. A., Čapková, P., Hatjisymeon, K., Fraanje, J. & Schenk, H. (1994). *Acta Cryst.* B. Submitted.

De Ridder, D. J. A., Fraanje, J., Goubitz, K. & Schenk, H. (1994). *Acta Cryst.* B. Submitted.

De Ridder, D. J. A., Goubitz, K. & Schenk, H. (1990). *Acta Cryst.* C**46**, 2200–2202.

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

Fehr, C., Galindo, J., Haubrichs, R. & Perret, R. (1989). *Helv. Chim. Acta*, **72**, 1537–1553.

Hall, S. R. & Stewart, J. M. (1990). Editors. *Xtal*3.0 *Reference Manual*. Univs. of Western Australia, Australia, and Maryland, USA.

Hummel, W., Hauser, J. & Bürgi, H.-B. (1990). *J. Mol. Graphics*, **8**, 214–220.

Lenselink, W. (1991). PFW-Amersfoort, The Netherlands. Private communication.

Walker, N. & Stuart, D. (1983). *Acta Cryst.* A**39**, 158–166.

Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564.

Acta Cryst. (1994). C**50**, 1966–1967

Honokiol

Michael J. Fullmer, R. Curtis Haltiwanger,
Nelson Troupe and Drake S. Eggleston

*SmithKline Beecham Pharmaceuticals,
709 Swedeland Road, King of Prussia, PA 19406, USA*

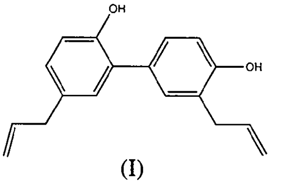
(*Received* 18 *February* 1994; *accepted* 23 *May* 1994)

Abstract

Alcoholic extracts of magnolia tree bark and seeds have been shown to contain several phenolic constituents, including honokiol (3′,5-di-2-propenyl-[1,1′-biphenyl]-2,4′-diol), $C_{18}H_{18}O_2$, the structure of which was established previously by spectroscopic methods. We report here a crystal structure determination of honokiol and demonstrate that the rings of its biphenyl core adopt a non-planar orientation. Both hydroxyl substituents participate in intermolecular hydrogen bonding with O···O distances near 2.8 Å.

Comment

The asymmetrically substituted diallylic dihydroxy-biphenyl compound honokiol was first isolated from magnolia tree bark by Fujita, Itokawa & Sashida (1973) and subsequently reported again as having been isolated from the seeds of *Magnolia grandiflora L.*, its structure having been determined by spectroscopic methods (El-Feraly & Li, 1978). During the course of fractionating constituents of a hexane extract of the pods of *Magnolia tripetala*, the title molecule (I) was reisolated.



(I)

In the crystallographic structure (Fig. 1), the biphenyl system adopts a non-planar orientation with a dihedral angle between the ring planes of 57.14 (1)°. Each hydroxyl group is hydrogen bonded intermolecularly to its counterpart along the *x* axis, as may be seen in Fig. 2. Metrical details of these interactions are: O1—O10 2.806 (2), HO1···O10 1.76 (4) Å, O1—HO1···O10 175 (3)°; O10—O1 2.833 (2), HO10···O1 1.97 (4) Å,

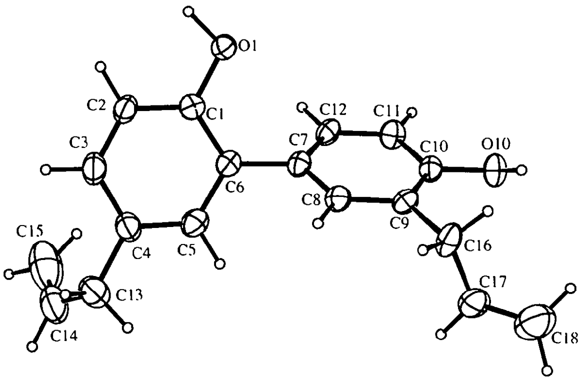


Fig. 1. An *ORTEP*II (Johnson, 1976) diagram of the honokiol structure. Non-H atoms are illustrated as principal ellipses at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

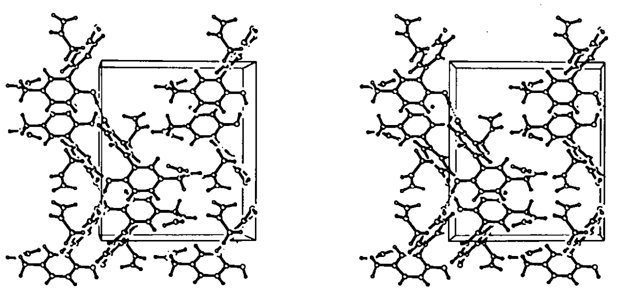


Fig. 2. A stereoscopic illustration of the unit-cell packing in the structure of honokiol. Hydrogen bonds are illustrated as thin lines.

O10—HO10···O1 155 (3)°. The structure of magnolol, a related diallylic dihydroxybiphenyl has been reported by Wang, Cheng, Lee & Chen (1982).

Experimental

Honokiol was isolated from a hexane extract of the pods of *Magnolia tripetala*; crystals were grown by slow evaporation from a mixture of methylene chloride and hexane.

Crystal data

$C_{18}H_{18}O_2$
$M_r = 266.34$
Monoclinic
$P2_1/c$
$a = 12.572$ (3) Å
$b = 14.442$ (3) Å
$c = 7.916$ (1) Å
$\beta = 94.46$ (1)°
$V = 1432.9$ (8) Å^3
$Z = 4$
$D_x = 1.235$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 15$–13°
$\mu = 0.074$ mm^{-1}
$T = 223$ K
Prism
0.70 × 0.40 × 0.40 mm
Colorless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
2904 measured reflections
1876 independent reflections
1218 observed reflections
[$I > 3.0\sigma(I)$]

$R_{\text{int}} = 0.033$
$\theta_{\text{max}} = 22.43°$
$h = -13 \rightarrow 13$
$k = 0 \rightarrow 15$
$l = -8 \rightarrow 3$
3 standard reflections
frequency: 180 min
intensity variation: −1.11%

Refinement

Refinement on F
$R = 0.041$
$wR = 0.049$
$S = 1.531$
1218 reflections
190 parameters
H atoms refined with $U = 1.3 \times U_{\text{eq}}$(C or O)
$w = 4F_o^2/[\sigma^2(F_o^2) + 0.0016F_o^4]$
$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.210$ e Å^{-3}
$\Delta\rho_{\text{min}} = -0.177$ e Å^{-3}
Extinction correction: isotropic (Zachariasen, 1963)
Extinction coefficient: 0.15 (1) × 10^{-5}
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)

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

	x	y	z	U_{eq}
O1	0.0484 (2)	0.1640 (1)	0.4192 (2)	0.030 (1)
O10	0.0293 (2)	−0.1778 (1)	−0.0745 (2)	0.031 (1)
C1	0.1581 (2)	0.1591 (2)	0.4552 (3)	0.025 (1)
C2	0.2098 (2)	0.2218 (2)	0.5661 (3)	0.032 (2)
C3	0.3188 (3)	0.2187 (2)	0.5976 (4)	0.037 (2)
C4	0.3796 (2)	0.1523 (2)	0.5204 (4)	0.033 (2)
C5	0.3260 (2)	0.0901 (2)	0.4108 (4)	0.032 (2)
C6	0.2150 (2)	0.0913 (2)	0.3745 (3)	0.025 (1)
C7	0.1641 (2)	0.0231 (2)	0.2536 (3)	0.023 (1)
C8	0.1962 (2)	0.0162 (2)	0.0900 (3)	0.027 (1)
C9	0.1524 (2)	−0.0492 (2)	−0.0266 (3)	0.025 (1)
C10	0.0753 (2)	−0.1086 (2)	0.0277 (3)	0.024 (1)
C11	0.0415 (2)	−0.1029 (2)	0.1893 (3)	0.029 (2)
C12	0.0858 (2)	−0.0372 (2)	0.3013 (3)	0.026 (1)
C13	0.4994 (3)	0.1495 (2)	0.5530 (5)	0.052 (2)
C14	0.5414 (3)	0.1224 (3)	0.7282 (5)	0.064 (2)
C15	0.4855 (4)	0.1014 (3)	0.8540 (5)	0.082 (3)
C16	0.1878 (3)	−0.0531 (2)	−0.2054 (3)	0.034 (2)
C17	0.2567 (3)	−0.1342 (3)	−0.2362 (4)	0.045 (2)
C18	0.2428 (3)	−0.1920 (3)	−0.3623 (5)	0.066 (2)

Table 2. *Selected bond lengths* (Å)

O1—C1	1.389 (3)	C7—C12	1.388 (3)
O10—C10	1.384 (3)	C8—C9	1.404 (3)
C1—C2	1.387 (3)	C9—C10	1.387 (3)
C1—C6	1.396 (3)	C9—C16	1.517 (3)
C2—C3	1.374 (4)	C10—C11	1.382 (3)
C3—C4	1.397 (4)	C11—C12	1.386 (3)
C4—C5	1.386 (4)	C13—C14	1.497 (5)
C4—C13	1.508 (4)	C14—C15	1.299 (5)
C5—C6	1.403 (4)	C16—C17	1.488 (4)
C6—C7	1.483 (3)	C17—C18	1.303 (4)
C7—C8	1.390 (3)		

The experimental crystal was mounted on a glass fiber with Paratone-N oil and flash cooled in a stream of N_2 gas. Intensity data were collected using an Mo rotating-anode source. Corrections were applied for a slight decay in diffraction intensity during the experiment. The positions and isotropic temperature factors of H atoms attached to C atoms were assigned from geometrical considerations. The positions of the hydroxyl H atoms were located from difference Fourier maps and were refined along with their isotropic temperature factors.

Data collection: CAD-4 diffractometer software (Enraf–Nonius, 1977). Cell refinement: CAD-4 diffractometer software. Data reduction: *MolEN PROCESS* (Fair, 1990). Program(s) used to solve structure: *MULTAN*80 (Main *et al.*, 1980). Program(s) used to refine structure: *MolEN LSFM*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *BTABLE*, *PTABLE* and *CIF IN* in *MolEN*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry, including bond distances and angles involving H atoms, and torsion angles have been deposited with the IUCr (Reference: CR1143). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

El-Feraly, F. S. & Li, W. S. (1978). *J. Nat. Prod.* **41**, 442–449.
Enraf–Nonius (1977). *CAD-4 Operations Manual.* Enraf–Nonius, Delft, The Netherlands.
Fair, C. K. (1990). *MolEN. An Interactive Intelligent System for Crystal Structure Analysis.* Enraf–Nonius, Delft, The Netherlands.
Fujita, M., Itokawa, H. & Sashida, Y. (1973). *Yakugaku Zasshi*, **93**, 422–426.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Main, P., Fiske, S. J., Hull, S. E., Lessinger, L., Germain, G., Declercq, J.-P. & Woolfson, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.
Wang, Y., Cheng, M.-C., Lee, J.-S. & Chen, F.-C. (1982). *J. Chin. Chem. Soc.* **30**, 215.
Zachariasen, W. H. (1963). *Acta Cryst.* **16**, 1139–1144.