Tableau 1. *Coordonnées atomiques et facteurs d'agitation thermique isotropes équivalents* (Å^2)

$$U_{éq} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{éq}$
N(1)	0,9327 (5)	0,1924 (2)	0,6617 (6)	0,044 (1)
C(2)	1,0325 (6)	0,1441 (2)	0,6763 (7)	0,038 (1)
C(3)	1,2033 (6)	0,1411 (2)	0,6687 (8)	0,044 (1)
C(4)	1,2840 (6)	0,1924 (2)	0,6479 (7)	0,043 (1)
C(5)	1,1885 (7)	0,2435 (2)	0,6369 (8)	0,044 (1)
C(6)	1,0157 (6)	0,2418 (2)	0,6424 (7)	0,041 (1)
N(7)	0,9278 (5)	0,0955 (2)	0,6959 (7)	0,047 (1)
C(8)	0,9778 (7)	0,0395 (2)	0,7241 (8)	0,046 (1)
C(9)	0,8320 (7)	0,0016 (2)	0,7468 (8)	0,043 (1)
N(10)	0,6796 (5)	0,0268 (2)	0,7465 (6)	0,046 (1)
C(11)	0,5515 (7)	−0,0089 (2)	0,7669 (8)	0,052 (3)
C(12)	0,5784 (6)	−0,0676 (2)	0,7939 (8)	0,047 (1)
N(13)	0,7308 (5)	−0,0923 (2)	0,7923 (7)	0,056 (1)
C(14)	0,8599 (7)	−0,0571 (2)	0,7725 (8)	0,051 (1)
O(15)	1,1242 (5)	0,0196 (1)	0,7325 (6)	0,058 (1)
C(16)	1,4695 (7)	0,1921 (3)	0,6344 (9)	0,071 (3)
C(17)	0,9087 (7)	0,2962 (2)	0,6324 (8)	0,058 (3)
C(18)	0,4357 (7)	−0,1058 (3)	0,8211 (9)	0,072 (3)

Tableau 2. *Paramètres géométriques* (Å, °)

N(1)—C(2)	1,348 (7)	C(8)—C(9)	1,497 (8)
N(1)—C(6)	1,348 (7)	C(8)—O(15)	1,221 (7)
C(2)—C(3)	1,363 (7)	C(9)—N(10)	1,331 (7)
C(2)—N(7)	1,431 (7)	C(9)—C(14)	1,379 (7)
C(3)—C(4)	1,379 (8)	N(10)—C(11)	1,349 (7)
C(4)—C(5)	1,389 (8)	C(11)—C(12)	1,380 (7)
C(4)—C(16)	1,493 (8)	C(12)—N(13)	1,330 (7)
C(5)—C(6)	1,371 (8)	C(12)—C(18)	1,494 (8)
C(6)—C(17)	1,503 (8)	N(13)—C(14)	1,347 (7)
N(7)—C(8)	1,349 (6)		
C(2)—N(1)—C(6)	115,1 (4)	N(7)—C(8)—C(9)	112,9 (5)
N(1)—C(2)—C(3)	126,3 (5)	N(7)—C(8)—O(15)	126,2 (5)
N(1)—C(2)—N(7)	108,9 (4)	C(9)—C(8)—O(15)	121,0 (4)
C(3)—C(2)—N(7)	124,8 (5)	C(8)—C(9)—N(10)	117,6 (4)
C(2)—C(3)—C(4)	117,2 (5)	C(8)—C(9)—C(14)	120,2 (5)
C(3)—C(4)—C(5)	118,8 (5)	N(10)—C(9)—C(14)	122,2 (5)
C(3)—C(4)—C(16)	120,0 (5)	C(9)—N(10)—C(11)	115,8 (4)
C(5)—C(4)—C(16)	121,3 (5)	N(10)—C(11)—C(12)	122,4 (5)
C(4)—C(5)—C(6)	119,5 (5)	C(11)—C(12)—N(13)	121,1 (5)
N(1)—C(6)—C(5)	123,2 (5)	C(11)—C(12)—C(18)	121,2 (5)
N(1)—C(6)—C(17)	115,8 (5)	N(13)—C(12)—C(18)	117,7 (5)
C(5)—C(6)—C(17)	121,1 (5)	C(12)—N(13)—C(14)	117,0 (4)
C(2)—N(7)—C(8)	128,7 (4)	C(9)—C(14)—N(13)	121,4 (5)

Plusieurs cristaux ont été utilisés au cours de l'étude structurale. Tous se sont avérés de qualité très médiocre. La structure a été résolue avec le programme *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) et la figure a été réalisée avec le programme *ORTEP*II (Johnson, 1976). Tous les programmes utilisés appartiennent au système *SDP* (B. A. Frenz & Associates, Inc., 1982). Les coordonnées des atomes d'hydrogène n'ont pas été affinées en raison du nombre insuffisant de réflexions observées.

Les listes des facteurs de structure, des facteurs d'agitation thermique anisotrope, des coordonnées des atomes d'hydrogène, des distances C—H et N—H, des angles de torsion, des distances interatomiques intermoléculaires et des distances des atomes aux plans moyens ont été déposées aux archives de l'UICr (Référence: PA1089). On peut en obtenir des copies en s'adressant à: The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.

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Crystal Studies of Musk Compounds. XIII.† Molecular Structures of 6-Formyl-1,1,2,4,4,7-hexamethyltetralin (1) and 6-Formyl-1,1,4,4,5,7-hexamethyltetralin (2)

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(*Received* 4 *January* 1994; *accepted* 9 *March* 1994)

Abstract

The crystal structures of the title compounds (1,1,2,4,4,7-hexamethyl- and 1,1,4,4,5,7-hexamethyl-1,2,3,4-tetrahydro-6-naphthalenecarbaldehyde, both musks of formula $C_{17}H_{24}O$), have been determined by X-ray diffraction. The non-aromatic ring adopts a half-chair conformation with the diad axis passing through the midpoint of the C2—C3 bond and that of the ring-fusion bond C9—C10. The formyl groups in both compounds show disorder, each with two partially resolved O atoms. With respect to the aromatic ring, the two conformations of the formyl groups differ by approximately 180°. Compound (2) also shows disorder in the cyclohexene ring. The possible muskiness for the two observed conformations of the formyl group is discussed.

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† This work forms part of a thesis by De Ridder (1992).

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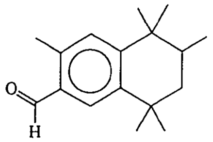
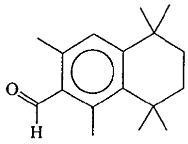
Acta Crystallographica Section C
ISSN 0108-2701 © 1994

Comment

The title compounds are lower homologues of Musk Tonalid (6-acetyl-1,1,2,4,4,7-hexamethyltetralin), the crystal structure of which has been described (De Ridder, Goubitz & Schenk, 1990). Compound (1) is the formyl equivalent of Musk Tonalid and is a musk (Lenselink, 1991). It is isomeric with compound (2), which is also a strong musk (Fehr, Galindo, Haubrichs & Perret, 1989).



(1)



(2)

In general, formyl musk compounds have a more persistent musk odour than the corresponding acetyl musks, but they have the disadvantage of being phototropic in the solid state, turning bright yellow on exposure to sunlight.

In order to be consistent within the family of the tetralin musks the numbering scheme applied to Musk Tonalid and its precursor (De Ridder, Goubitz & Schenk, 1990) and the three nitro compounds (De Ridder, Fraanje, Goubitz & Schenk, 1994) has been maintained (Figs. 1 and 2).

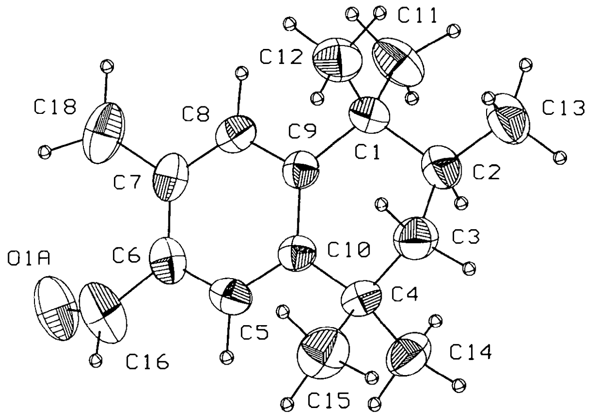


Fig. 1. *PEANUT* (Hummel, Hauser & Bürgi, 1990) drawing of compound (1) (with atom O1*A*) showing the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level; the H atoms are spheres of arbitrary size and are not labelled.

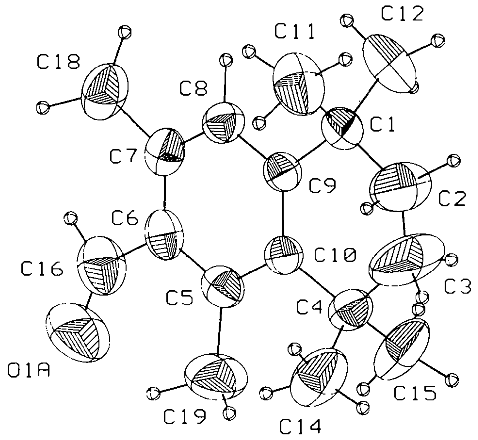


Fig. 2. *PEANUT* drawing of compound (2) (with atom O1*A*) showing the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level; the H atoms are spheres of arbitrary size and are not labelled.

In both compounds the molecules show disorder in the formyl substituent; two positions for the O atom were introduced and their population parameters refined. In (1) the O atom nearest to the aromatic methyl group refined to a population parameter of 0.57; in (2) the O atom nearest to the aromatic methyl group attached to C5 refined to a population parameter of 0.69. In Figs. 1 and 2 the molecules with the highest population parameter for the O atom (O1*A*) are shown [molecules (1*A*) and (2*A*)]; in the other configuration the formyl group is rotated by roughly 180° about C6—C16 with respect to the configuration shown. The cyclohexene ring in (2) shows the same type of disorder as discussed by De Ridder, Fraanje, Goubitz & Schenk (1994). This can be seen when the distances of atoms C2 and C3 from the plane through C1, C9, C10 and C4 are compared: −0.356 (7) and 0.345 (7) Å for (1), which shows no disorder, and −0.107 (9) and 0.058 (11) Å for (2). In the latter compound this disorder further manifests itself by relatively high displacement factors for C2 and C3, with deviations of the bond distances and angles involving these atoms. This manifestly high disorder combined with the generally poor quality of the crystals of this type of compound is reflected in the high *R* values.

In (1) the methyl group attached to C2 is found to be in the equatorial position, analogous to the tetralin compounds described in the papers mentioned above. The aromatic ring is essentially planar in both compounds, the maximum deviation of a ring atom from the best plane being 0.010 (4) for (1) and 0.013 (4) Å for (2).

The zero position of the angle between the planes formed by the atoms of the acyl substituent and the aromatic ring, respectively, is defined when the O atom in the plane of the phenyl ring faces the methyl group at C7 (such that the torsion angle C7—C6—C16—O is zero). For the acetyl compounds in preceding papers the first plane has been calculated considering the three non-H atoms it comprises, for the formyl compounds in the present paper the plane was defined by the atoms C6, C16 and O1. The angle in (1*A*) [23.2 (9)°] and in (2*B*) [−18 (1)°] compares very well to that of Musk Tonalid [22.6 (1)°; De Ridder, Goubitz & Schenk, 1990]. The angles for the molecules (1*B*) and (2*A*) are −170 (1) and −164.6 (7)°, respectively.

The dimensions of a triangle defined by the two quaternary C atoms C1 and C4 of the non-aromatic ring and the C(sp^2) atom (C16) of the formyl group compare very well to the values observed in Musk Tonalid (De Ridder, Goubitz & Schenk, 1990); the distance C1···C4 is 3.078 (5) in (1) and 3.057 (5) Å in (2) compared with 3.048 (10) Å in Musk Tonalid. The other distances are: C1···C16 5.802 (7), 5.789 (6) and 5.845 (12) Å and C4···C16 4.948 (7), 5.115 (6) and 5.011 (13) Å in (1), (2) and Musk Tonalid, respectively. However, this molecular descriptor does not take into account that there are two orientations found for the formyl group in the crystal in contrast to only one orientation for the acetyl group in Musk Tonalid or other bicyclic musk compounds (*cf.* indan compounds in De Ridder, Čapková, Hatjisymeon, Fraanje & Schenk, 1994). Since it is unknown whether both orientations of the formyl group can cause musk odour and in the absence of any knowledge of the receptor site, the argument for a better descriptor to correlate the structure to muskiness remains undecided. If the position of the O atom of an acetyl group is assumed to be the correct one with respect to the receptor site and considering the fact that one of the O atoms of a nitro group attached to the aromatic ring at the same position in nitro-musk compounds is approximately at the same place, there is reason to assume that only the formyl group with its O atom facing the methyl group at C7 will cause musk odour. Again it has to be mentioned that the dimensions of this triangle may be a necessary, but not the only, condition for muskiness.

Experimental

Compound (1) was prepared (at PFW-Amersfoort) according to a similar procedure to that described by Carpenter, Easter & Wood (1957). Compound (2) was prepared (at Firmenich) according to the literature procedure (Fehr, Galindo, Haubrichs & Perret, 1989). A sample of the crystals of (2) was recrystallized by slow evaporation from ethanol. The crystals were of poor quality. Owing to the high volatility and the phototropic properties of these compounds, the crystals were analysed at reduced temperature within an open nitrogen gas stream.

Compound (1)

Crystal data

$C_{17}H_{24}O$
$M_r = 244.38$
Monoclinic
$P2_1/n$
$a = 8.616$ (3) Å
$b = 10.435$ (2) Å
$c = 16.162$ (4) Å
$\beta = 90.63$ (3)°
$V = 1453.0$ (7) Å^3
$Z = 4$
$D_x = 1.115$ Mg m^{-3}

Cu *Kα* radiation
$\lambda = 1.5418$ Å
Cell parameters from 23 reflections
$\theta = 25.1$–$33.1°$
$\mu = 0.479$ mm^{-1}
$T = 245$ (1) K
Block
$0.60 \times 0.35 \times 0.15$ mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: empirical (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.66$, $T_{\max} = 1.61$
2680 measured reflections
2463 independent reflections
1520 observed reflections [$I > 2.5\sigma(I)$]

$\theta_{\max} = 64.87°$
$h = -10 \rightarrow 10$
$k = 0 \rightarrow 12$
$l = -19 \rightarrow 0$
2 standard reflections
frequency: 60 min
intensity variation: none

Refinement

Refinement on F
$R = 0.064$
$wR = 0.084$
$S = 0.221$
1520 reflections
271 parameters
$w = 1/(6.092 + F_o + 0.0072F_o^2)$
$(\Delta/\sigma)_{\max} = 0.252$
$\Delta\rho_{\max} = 0.413$ e Å^{-3}
$\Delta\rho_{\min} = -0.217$ e Å^{-3}

Extinction correction: Zachariasen (1967)
Extinction coefficient: $8\ (11) \times 10^{-7}$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Compound (2)

Crystal data

$C_{17}H_{24}O$
$M_r = 244.38$
Monoclinic
$P2_1/c$
$a = 10.366$ (1) Å
$b = 8.715$ (1) Å
$c = 15.984$ (2) Å
$\beta = 95.630$ (9)°
$V = 1437.0$ (3) Å^3
$Z = 4$
$D_x = 1.13$ Mg m^{-3}

Cu *Kα* radiation
$\lambda = 1.5418$ Å
Cell parameters from 23 reflections
$\theta = 40.0$–$43.8°$
$\mu = 0.484$ mm^{-1}
$T = 252$ (1) K
Block
$0.35 \times 0.25 \times 0.15$ mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: empirical (*DIFABS*; Walker & Stuart, 1983)
$T_{\min} = 0.45$, $T_{\max} = 1.34$
2671 measured reflections
2428 independent reflections
2053 observed reflections [$I > 2.5\sigma(I)$]

$\theta_{\max} = 64.84°$
$h = -11 \rightarrow 12$
$k = 0 \rightarrow 10$
$l = -18 \rightarrow 0$
2 standard reflections
frequency: 60 min
intensity variation: none

Refinement

Refinement on F
$R = 0.099$
$wR = 0.117$
$S = 0.235$
2053 reflections
241 parameters
$w = 1/(7.52 + F_o + 0.0046F_o^2)$

$(\Delta/\sigma)_{\max} = 0.389$
$\Delta\rho_{\max} = 0.401$ e Å^{-3}
$\Delta\rho_{\min} = -0.517$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

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	$U_{\rm eq}$
Compound (1)				
C1	−0.0120 (4)	0.8032 (3)	0.2876 (2)	0.043 (2)
C2	0.0859 (5)	0.9269 (4)	0.2841 (3)	0.056 (2)
C3	0.1482 (5)	0.9657 (4)	0.3670 (3)	0.059 (3)
C4	0.2576 (4)	0.8689 (3)	0.4068 (2)	0.043 (2)
C5	0.2556 (4)	0.6352 (4)	0.4443 (2)	0.046 (2)
C6	0.2037 (4)	0.5090 (3)	0.4408 (2)	0.048 (2)
C7	0.0796 (4)	0.4796 (3)	0.3881 (2)	0.047 (2)
C8	0.0156 (4)	0.5765 (4)	0.3412 (2)	0.045 (2)
C9	0.0697 (4)	0.7045 (3)	0.3434 (2)	0.038 (2)
C10	0.1919 (4)	0.7346 (3)	0.3976 (2)	0.037 (2)
C11	−0.0270 (6)	0.7503 (5)	0.1994 (3)	0.069 (3)
C12	−0.1747 (5)	0.8268 (5)	0.3218 (3)	0.065 (3)
C13	0.0019 (6)	1.0396 (5)	0.2420 (3)	0.072 (3)
C14	0.4195 (5)	0.8741 (4)	0.3694 (3)	0.059 (3)
C15	0.2739 (7)	0.9059 (5)	0.4992 (3)	0.071 (3)
C16	0.2836 (9)	0.4135 (6)	0.4911 (4)	0.085 (4)
C18	0.0128 (7)	0.3451 (4)	0.3817 (3)	0.074 (3)
O1*A*†	0.2976 (9)	0.3015 (5)	0.4870 (4)	0.085 (4)
O1*B*†	0.368 (1)	0.427 (1)	0.5383 (9)	0.108 (9)
Compound (2)				
C1	0.8528 (3)	0.7386 (4)	0.4081 (2)	0.053 (2)
C2	0.9362 (5)	0.8077 (8)	0.3465 (4)	0.111 (4)
C3	0.9007 (5)	0.925 (1)	0.3028 (6)	0.191 (8)
C4	0.7709 (4)	0.9932 (4)	0.2824 (2)	0.055 (2)
C5	0.5434 (3)	0.9655 (4)	0.3336 (2)	0.053 (2)
C6	0.4584 (3)	0.9024 (4)	0.3890 (2)	0.053 (2)
C7	0.5021 (3)	0.7905 (4)	0.4473 (2)	0.053 (2)
C8	0.6283 (3)	0.7444 (4)	0.4493 (2)	0.052 (2)
C9	0.7158 (3)	0.8043 (4)	0.3968 (2)	0.044 (2)
C10	0.6744 (3)	0.9191 (4)	0.3382 (2)	0.044 (2)
C11	0.8512 (5)	0.5652 (6)	0.3938 (4)	0.087 (3)
C12	0.9146 (5)	0.7703 (7)	0.4974 (3)	0.087 (3)
C14	0.7342 (7)	0.9701 (8)	0.1887 (3)	0.100 (4)
C15	0.7862 (7)	1.1658 (6)	0.3002 (4)	0.100 (4)
C16	0.3220 (5)	0.9529 (6)	0.3881 (3)	0.081 (3)
C18	0.4170 (5)	0.7170 (6)	0.5085 (3)	0.076 (3)
C19	0.4870 (5)	1.0834 (7)	0.2712 (4)	0.097 (4)
O1*A*‡	0.2540 (5)	1.0239 (8)	0.3382 (4)	0.121 (5)
O1*B*‡	0.237 (1)	0.890 (2)	0.416 (1)	0.14 (1)

† Population parameters: O1*A* 0.57, O1*B* 0.43.
‡ Population parameters: O1*A* 0.69, O1*B* 0.31.

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

	(1)	(2)
C1—C2	1.543 (5)	1.500 (7)
C1—C9	1.534 (5)	1.525 (5)
C1—C11	1.533 (6)	1.528 (6)
C1—C12	1.533 (6)	1.530 (6)
C2—C3	1.493 (6)	1.27 (1)
C2—C13	1.536 (7)	-
C3—C4	1.519 (6)	1.478 (7)
C4—C10	1.518 (5)	1.545 (5)
C4—C14	1.527 (5)	1.522 (6)
C4—C15	1.548 (6)	1.536 (7)
C5—C6	1.391 (5)	1.420 (5)
C5—C10	1.392 (5)	1.412 (5)
C5—C19	-	1.509 (7)
C6—C7	1.394 (5)	1.394 (5)
C6—C16	1.455 (7)	1.479 (6)
C7—C8	1.376 (5)	1.367 (5)
C7—C18	1.521 (6)	1.521 (6)
C8—C9	1.415 (5)	1.397 (5)
C9—C10	1.398 (5)	1.408(4)
C16—O1*A*	1.176 (8)	1.186 (8)
C16—O1*B*	1.06 (1)	1.16 (2)
C2—C1—C9	109.6 (3)	111.2 (3)
C2—C1—C11	107.9 (3)	107.3 (4)
C2—C1—C12	112.4 (3)	108.9 (4)
C9—C1—C11	109.8 (3)	110.9 (3)
C9—C1—C12	108.1 (3)	110.1 (3)
C11—C1—C12	109.0 (3)	108.4 (4)
C1—C2—C3	112.6 (3)	122.0 (5)
C1—C2—C13	113.7 (4)	-
C3—C2—C13	110.6 (4)	-
C2—C3—C4	114.5 (3)	130.7 (6)
C3—C4—C10	110.1 (3)	109.4 (4)
C3—C4—C14	112.0 (3)	107.3 (5)
C3—C4—C15	107.0 (3)	106.1 (5)
C10—C4—C14	109.6 (3)	113.6 (4)
C10—C4—C15	110.8 (3)	111.3 (4)
C14—C4—C15	107.4 (3)	108.8 (4)
C6—C5—C10	123.9 (3)	120.6 (3)
C6—C5—C19	-	116.9 (3)
C10—C5—C19	-	122.5 (4)
C5—C6—C7	118.5 (3)	120.5 (3)
C5—C6—C16	118.4 (4)	122.0 (3)
C7—C6—C16	123.1 (4)	117.5 (4)
C6—C7—C8	118.4 (3)	118.0 (3)
C6—C7—C18	122.2 (4)	123.6 (3)
C8—C7—C18	119.5 (4)	118.4 (3)
C7—C8—C9	123.4 (3)	123.6 (3)
C1—C9—C8	118.0 (3)	116.1 (3)
C1—C9—C10	123.7 (3)	124.4 (3)
C8—C9—C10	118.2 (3)	119.5 (3)
C4—C10—C5	119.4 (3)	121.6 (3)
C4—C10—C9	123.0 (3)	120.5 (3)
C5—C10—C9	117.6 (3)	117.9 (3)
C6—C16—O1*A*	134.2 (6)	131.8 (5)
C6—C16—O1*B*	129.0 (9)	127.9 (9)

The structures were determined by direct methods using *Xtal SIMPEL* (Hall & Stewart, 1990). All H atoms were placed in geometrically calculated positions and refined in the structure-factor calculations as riding atoms. For compound (1) the U value of the H atom attached to C16 was kept fixed at 0.06 Å^2. The displacement parameters of all H atoms in (2) were kept fixed at 0.08 Å^2 and the angles of the H atoms attached to C2 and C3 were restrained at 109°. H16*A* and H16*B* were not refined. In the first stage of the refinement of each structure the displacement parameter of the O atom was kept fixed and the population parameter was refined. After convergence of the population parameter, it was kept fixed and the O atoms were refined anisotropically.

For both compounds, data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CELCON* comparable to *Xtal LATCON* (Hall & Stewart, 1990); data reduction: *Xtal SORTRF* and *Xtal ADDREF*; program(s) used to solve structures: *Xtal SIMPEL*; program(s) used to refine structures: *Xtal CRYLSQ*; molecular graphics: *PEANUT* (Hummel, Hauser & Bürgi, 1990); software used to prepare material for publication: *Xtal BONDLA* and *Xtal CIFIO*.

The authors are grateful to Dr A. M. Cohen and Drs W. Lenselink of PFW-Amersfoort (The Netherlands) for providing the crystals of compound (1) and Dr C. Fehr 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.

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Honokiol

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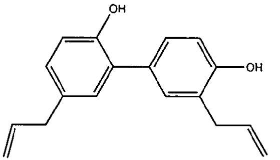
(*Received* 18 *February* 1994; *accepted* 23 *May* 1994)

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 dihydroxybiphenyl 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,

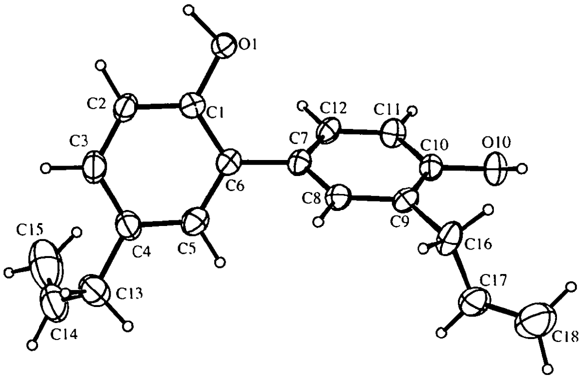


Fig. 1. An *ORTEP*II (Johnson, 1976) diagram of the honokiol structure. Non-H atoms are illustrated as principal ellipses at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

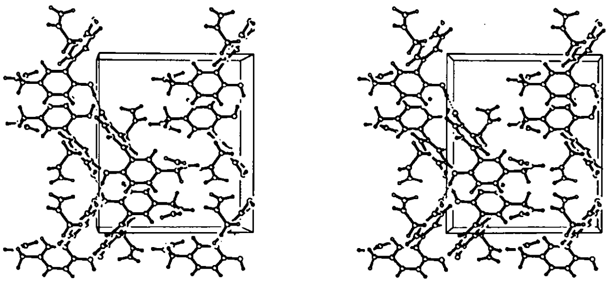


Fig. 2. A stereoscopic illustration of the unit-cell packing in the structure of honokiol. Hydrogen bonds are illustrated as thin lines.