C7—C8—C9	109.3 (1)	C7—C18—C19	94.2 (2)
C7—C8—C19	85.4 (1)	C8—C19—C18	94.8 (2)
C9—C8—C19	119.2 (2)		

Structure solution and refinement were performed using the *SDP* (Frenz, 1978) program package on a VAXII/730 computer. Molecular structures were plotted using the *PLUTO* program (Motherwell & Clegg, 1978).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71521 (28 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HA1052]

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2,2′-Di-*O*-acetyl-3,6;3′,6′-dianhydro-4,4′-dideoxy-α,α-trehalose

C. K. Lee and L. L. Koh

Department of Chemistry, Faculty of Science, National University of Singapore, Singapore 0511

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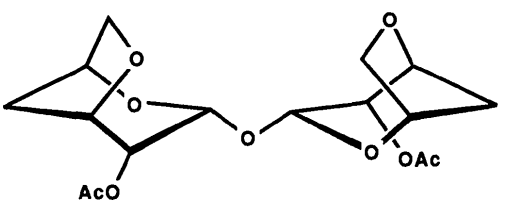
Abstract

The structure of 2,2′-di-*O*-acetyl-3,6;3′,6′-dianhydro-4,4′-dideoxy-α,α-trehalose (2-*O*-acetyl-3,6-anhydro-4-deoxy-α-D-*xylo*-hexopyranosyl 2-*O*-acetyl-3,6-anhydro-4-deoxy-α-D-*xylo*-hexopyranoside), $C_{16}H_{22}O_9$, is described. The molecule has approximate two-fold symmetry through O(1). Both pyranoid rings have distorted $^1C_4$ chair conformations and the five-membered anhydro rings have distorted ^4E conformations. The structure of the compound appears to show the absence of a sweet *A*H,*B* glucophore, which would explain the absence of sweetness in the unsubstituted derivative.

Comment

The Shallenberger *A*H,*B* theory of sweetness (Shallenberger & Acree, 1967) suggests that the fundamental unit of sweetness is an *A*H,*B* system, where *A* and *B* are electronegative atoms in suitable geometric proximity. The Kier extension to the *A*H,*B* concept (Kier, 1972) is that a third hydrophilic (γ) binding site, if present, will increase the intensity of the sweet taste. The ideal molecule for taste studies in sugars is probably α,α-trehalose. It contains two chemically equivalent glucopyranose residues in the most stable $^4C_1$ conformation, linked glycosidically through their reducing (anomeric) C atoms. Stability is high in the sugar and its derivatives because all the hydroxyl substituents are equatorially disposed. Because the interatomic distances are of great importance in determining sweetness, we have undertaken the X-ray crystal diffraction study of α,α-trehalose derivatives.

A *SHELXTL-Plus* (Sheldrick, 1990) *XP* plot of 2,2′-di-*O*-acetyl-3,6;3′,6′-dianhydro-4,4′-dideoxy-α,α-trehalose (Birch, Lee & Richardson, 1974) (1) with the atomic numbering scheme is shown in Fig. 1, and the molecular packing in the crystal is shown in Fig. 2. Like α,α-trehalose, the two glucopyranosyl residues of (1) have approximate C_2 symmetry but the structural differences between the two residues are much smaller. Differences are found in the torsion angles about the glycosidic O atom, especially those involving C(2) and C(2′) (Table 3), and in the conformation of the C(2) and C(2′) acetyl groups.



(1)

Bond lengths, bond angles and selected torsion angles are given in Tables 2 and 3. Bond lengths and angles agree well with those of methyl 3,6-anhydro-α-D-hexopyranosides (Lindberg, Lindberg & Svensson, 1973; Campbell & Harding, 1972), and most other pyranose sugars (Berman, Chu & Jeffrey, 1967). The O(1)—C(1) and O(1)—C(1′) bond lengths show systematic trends similar to those observed in other α-pyranose sugars (Berman, Chu & Jeffrey, 1967) but are shorter than those in α,α-trehalose (Brown, Rohrer, Berking, Beevers, Gould & Simpson, 1972; Taga, Senma & Osaki, 1972; Jeffrey & Nanni, 1985) and its 3,3-dideoxy derivative (Lee &

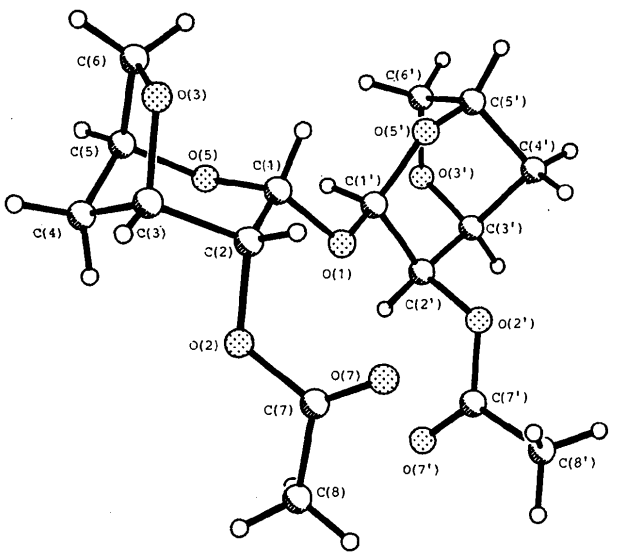


Fig. 1. Molecular conformation of 2,2′-di-*O*-acetyl-3,6;3′,6′-dianhydro-4,4′-dideoxy-α,α-trehalose.

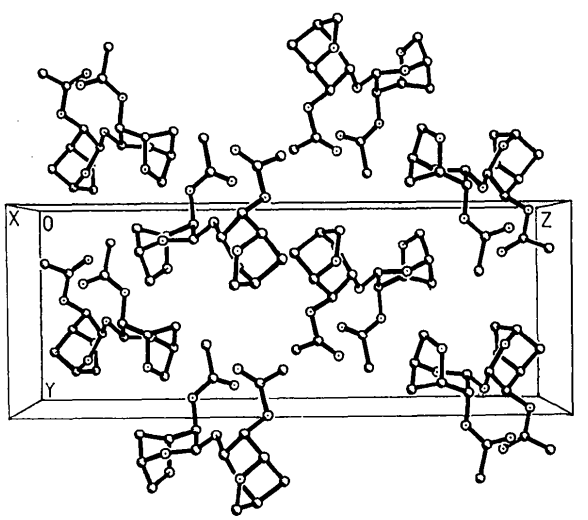


Fig. 2. Molecular packing in 2,2′-di-*O*-acetyl-3,6;3′,6′-dianhydro-4,4′-dideoxy-α,α-trehalose.

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

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

	x	y	z	U_{eq}
C(1)	0.1337 (8)	1.1587 (7)	0.3831 (3)	0.043 (2)
C(2)	0.2294 (8)	1.0526 (7)	0.4207 (3)	0.043 (2)
C(3)	0.3536 (8)	1.1439 (8)	0.4550 (3)	0.051 (2)
C(4)	0.2700 (8)	1.2636 (8)	0.4889 (3)	0.050 (2)
C(5)	0.2213 (9)	1.3670 (8)	0.4413 (3)	0.051 (3)
C(6)	0.3751 (9)	1.3731 (8)	0.4075 (3)	0.064 (3)
C(7)	0.0736 (9)	0.8327 (8)	0.4471 (3)	0.052 (3)
C(8)	−0.0536 (11)	0.7819 (9)	0.4874 (3)	0.082 (3)
O(1)	−0.0119 (5)	1.0871 (5)	0.3677 (2)	0.048 (2)
O(2)	0.1229 (5)	0.9775 (5)	0.4606 (2)	0.047 (2)
O(3)	0.4498 (5)	1.2259 (6)	0.4152 (2)	0.057 (2)
O(5)	0.0895 (5)	1.2986 (5)	0.4109 (2)	0.052 (2)
O(7)	0.1291 (7)	0.7629 (5)	0.4088 (2)	0.074 (2)
C(1′)	−0.1071 (8)	1.1653 (8)	0.3295 (3)	0.046 (2)
C(2′)	−0.2716 (9)	1.0891 (9)	0.3256 (3)	0.057 (3)
C(3′)	−0.3601 (10)	1.1440 (10)	0.2736 (4)	0.079 (4)
C(4′)	−0.2595 (12)	1.1069 (11)	0.2221 (3)	0.090 (4)
C(5′)	−0.1264 (10)	1.2241 (11)	0.2312 (3)	0.076 (3)
C(6′)	−0.2233 (10)	1.3621 (11)	0.2458 (4)	0.081 (4)
C(7′)	−0.3154 (12)	0.8382 (13)	0.3568 (5)	0.096 (5)
C(8′)	−0.2787 (12)	0.6736 (10)	0.3454 (5)	0.121 (5)
O(2′)	−0.2474 (7)	0.9283 (7)	0.3210 (2)	0.070 (2)
O(3′)	−0.3655 (6)	1.3056 (8)	0.2743 (3)	0.084 (2)
O(5′)	−0.0261 (5)	1.1723 (6)	0.2770 (2)	0.059 (2)
O(7′)	−0.3941 (13)	0.8796 (10)	0.3946 (5)	0.206 (6)

Koh, 1993). The small C(3)—C(4)—C(5) angles [98.6 (6) (unprimed), 97.8 (7)° (primed)], which are also observed in 3,6-anhydro-α-D-hexopyranoside derivatives (Lindberg, Lindberg & Svensson, 1973; Campbell & Harding, 1972; Isaac & Kennard, 1972), are a consequence of strain introduced by the *cis*-fused five-membered anhydro ring. This strain also causes the C(3)···C(5) and C(3)···C(5′) distances (~2.3 Å) to be shorter by ~0.2 Å than those found for an unbridged pyranose ring. The distances between the axial O(2) and H(4_{axial}), and O(2′) and H($4'_{axial}$) are also similarly narrowed (~2.5 Å).

Both the pyranosyl rings have $^1C_4$ conformations with torsion angles defined by the six ring bonds ranging in magnitude from 41.4 to 72.0°. These variations are significantly larger than those of unbridged pyranose rings and are probably because of the *cis*-fused five-membered ring. The torsion angles at C(1) [C(5)—O(5)—C(1)—C(2) and O(5)—C(1)—C(2)—C(3)] are nearly half those at the opposite atoms [C(4)] in both rings (Table 3). C(1) and C(4) and C(1′) and C(4′) are −0.52 (1) and 0.87 (1) Å, and −0.53 (1) and 0.90 (1) Å, respectively, from the least-square planes C(2)–C(3)–C(5)–O(5) and C(2′)–C(3′)–C(5′)–O(5′), respectively. The mean distance out of the plane for C(1) and C(4) of a glucopyranose residue is ~0.66 Å (Ramachandran, Ramakrishnan & Sasisekharan, 1963). The chair is, thus, flattened at C(1) and tends towards an envelope conformation, apparently to relieve the strain caused by a tendency for O(5) and C(2) to be pushed apart in the formation of the anhydro ring. The puckering parameters of the pyranose rings (Cremer & Pople, 1975) are given in Table 4.

The five-membered anhydro rings are the least flexible parts of the molecule. The rings have distorted ^4E conformations with C(4) and C(4′) lying 0.70 (1) and 0.72 (1) Å above the least-squares planes C(3)–O(3)–C(5)–C(6) and C(3′)–O(3′)–C(5′)–C(6′), respectively. The distortion is expressed by a non-zero torsion angle C(3)—O(3)—C(6)—C(5) of 4.9° (3.5° for the primed ring).

The sweet-taste mechanism involves an aqueous solution. Thus the dynamic interplay of hydrogen bonds between water molecules and those of a sweet compound could possibly affect the conformation of

Table 2. *Bond lengths* (Å) *and bond angles* (°) *in compound* (1) *and methyl-3,6-anhydro-α-D-hexopyranosides*

Compound (1)				Methyl-3,6-anhydro-α-D-hexopyranosides Galacto*	Gluco†
C(1)—C(2)	1.510 (9)	C(1′)—C(2′)	1.513 (10)	1.553 (3)	1.50 (3)
C(2)—C(3)	1.532 (9)	C(2′)—C(3′)	1.507 (12)	1.534 (4)	1.57 (3)
C(3)—C(4)	1.491 (10)	C(3′)—C(4′)	1.508 (13)	1.535 (4)	1.41 (4)
C(4)—C(5)	1.500 (10)	C(4′)—C(5′)	1.519 (13)	1.526 (3)	1.56 (3)
C(5)—C(6)	1.497 (10)	C(5′)—C(6′)	1.492 (13)	1.518 (4)	1.53 (4)
O(1)—C(1)	1.402 (8)	O(1)—C(1′)	1.378 (8)	1.374 (4)	1.38 (2)
O(2)—C(2)	1.442 (8)	O(2′)—C(2′)	1.431 (10)	1.432 (4)	1.50 (2)
O(3)—C(3)	1.425 (8)	O(3′)—C(3′)	1.421 (12)	1.429 (3)	1.50 (3)
O(3)—C(6)	1.444 (9)	O(3′)—C(6′)	1.439 (10)	1.449 (4)	1.44 (3)
O(5)—C(1)	1.442 (8)	O(5′)—C(1′)	1.408 (10)	1.449 (3)	1.40 (3)
O(5)—C(5)	1.433 (8)	O(5′)—C(5′)	1.434 (9)	1.449 (3)	1.49 (2)
O(2)—C(7)	1.373 (8)	O(2′)—C(7′)	1.286 (13)		
O(7)—C(7)	1.182 (9)	O(7′)—C(7′)	1.162 (16)		
C(1)—O(1)—C(1′)	115.6 (5)			114.9 (2)	115 (2)
C(1)—O(5)—C(5)	113.3 (5)	C(1′)—O(5′)—C(5′)	113.9 (9)	107.1 (2)	116 (2)
C(1)—C(2)—C(3)	109.6 (5)	C(1′)—C(2′)—C(3′)	109.8 (6)	108.9 (2)	108 (2)
C(2)—C(3)—C(4)	110.2 (6)	C(2′)—C(3′)—C(4′)	108.8 (7)	109.3 (2)	118 (2)
C(2)—O(2)—C(7)	117.1 (5)	C(2′)—O(2′)—C(7′)	119.9 (7)		
C(3)—C(4)—C(5)	98.6 (6)	C(3′)—C(4′)—C(5′)	97.8 (7)	97.7 (2)	100 (2)
C(3)—O(3)—C(6)	107.4 (5)	C(3′)—O(3′)—C(6′)	108.3 (6)	108.3 (2)	105 (2)
C(4)—C(5)—C(6)	101.2 (6)	C(4′)—C(5′)—C(6′)	101.5 (7)	101.8 (2)	97 (2)
O(1)—C(1)—C(2)	108.7 (5)	O(1)—C(1′)—C(2′)	109.1 (6)	108.0 (2)	108 (2)
O(1)—C(1)—O(5)	106.6 (5)	O(1)—C(1′)—O(5′)	109.2 (5)	107.1 (2)	108 (2)
O(2)—C(2)—C(1)	110.4 (5)	O(2′)—C(2′)—C(1′)	108.5 (6)	111.9 (2)	108 (2)
O(2)—C(2)—C(3)	107.6 (5)	O(2′)—C(2′)—C(3′)	108.8 (7)	107.4 (2)	103 (2)
O(2)—C(7)—O(7)	122.8 (7)	O(2′)—C(7′)—O(7′)	123.7 (11)		
O(2)—C(7)—C(8)	109.9 (2)	O(2′)—C(7′)—C(8′)	112.9 (9)		
O(3)—C(3)—C(2)	106.7 (6)	O(3′)—C(3′)—C(2′)	109.1 (7)	108.5 (2)	104 (2)
O(3)—C(3)—C(4)	104.7 (5)	O(3′)—C(3′)—C(4′)	104.0 (7)	104.8 (2)	104 (2)
O(3)—C(6)—C(5)	105.1 (6)	O(3′)—C(6′)—C(5′)	105.2 (7)	105.4 (2)	107 (2)
O(5)—C(1)—C(2)	113.0 (5)	O(5′)—C(1′)—C(2′)	113.0 (5)	112.8 (2)	116 (2)
O(5)—C(5)—C(4)	108.9 (5)	O(5′)—C(5′)—C(4′)	107.8 (7)	107.0 (2)	109 (2)
O(5)—C(5)—C(6)	112.9 (6)	O(5′)—C(5′)—C(6′)	113.0 (6)	112.8 (2)	111 (2)
O(7)—C(7)—C(8)	127.3 (7)	O(7′)—C(7′)—C(8′)	122.5 (11)		

* Campbell & Harding (1972).
† Lindberg, Lindberg & Svensson (1973).

Table 3. *Selected torsion angles* (°) *of compound* (1) *and the pyranose ring in* 3,6;1′,4′;3′,6′*-trianhydrosucrose*

				Pyranose ring of 3,6;1′4′;3′,6′-trianhydrosucrose*
Within the 3,6-anhydro-α-D-glucopyranoside rings of (1)				
C(1)—C(2)—C(3)—C(4)	57.3 (0.7)	C(1′)—C(2′)—C(3′)—C(4′)	59.1 (0.9)	58.5
C(1)—C(2)—C(3)—O(3)	−55.8 (0.7)	C(1′)—C(2′)—C(3′)—O(3′)	−53.8 (0.8)	
C(2)—C(3)—C(4)—C(5)	−70.5 (0.6)	C(2′)—C(3′)—C(4′)—C(5′)	−72.0 (0.9)	−67.3
C(2)—C(3)—O(3)—C(6)	92.0 (0.6)	C(2′)—C(3′)—O(3′)—C(6′)	89.7 (0.7)	
C(3)—C(4)—C(5)—C(6)	−45.5 (0.6)	C(3′)—C(4′)—C(5′)—C(6′)	−45.3 (0.8)	
C(3)—C(4)—C(5)—O(5)	73.6 (0.6)	C(3′)—C(4′)—C(5′)—O(5′)	73.7 (0.8)	70.2
C(4)—C(5)—C(6)—O(3)	32.1 (0.7)	C(4′)—C(5′)—C(6′)—O(3′)	31.4 (0.8)	
C(4)—C(5)—O(5)—C(1)	−64.8 (0.7)	C(4′)—C(5′)—O(5′)—C(1′)	−64.8 (0.8)	−68.8
C(5)—O(5)—C(1)—C(2)	46.3 (0.7)	C(5′)—O(5′)—C(1′)—C(2′)	46.7 (0.8)	55.0
C(5)—C(6)—O(3)—C(3)	−4.9 (0.7)	C(5′)—C(6′)—O(3′)—C(3′)	−3.5 (0.8)	
O(5)—C(1)—C(2)—C(3)	−41.4 (0.7)	O(5′)—C(1′)—C(2′)—C(3′)	−42.9 (0.8)	−49.1
Outside the 3,6-anhydro-α-D-glucopyranoside rings of (1)				
O(1)—C(1)—C(2)—C(3)	−159.5 (0.5)	O(1)—C(1′)—C(2′)—C(3′)	−164.5 (0.6)	
O(1)—C(1)—C(2)—O(2)	−41.1 (0.7)	O(1)—C(1′)—C(2′)—O(2′)	−45.7 (0.7)	
O(1)—C(1)—O(5)—C(5)	165.6 (0.5)	O(1)—C(1′)—O(5′)—C(5′)	168.3 (0.6)	
O(2)—C(2)—C(3)—C(4)	−62.8 (0.7)	O(2′)—C(2′)—C(3′)—C(4′)	−59.4 (0.9)	
O(2)—C(2)—C(3)—O(3)	−175.8 (0.5)	O(2′)—C(2′)—C(3′)—O(3′)	−172.4 (0.6)	
O(5)—C(1)—O(1)—C(1′)	62.9 (0.6)	O(5′)—C(1′)—O(1)—C(1)	66.6 (0.7)	
C(2)—C(1)—O(1)—C(1′)	−175.0 (0.5)	C(2′)—C(1′)—O(1)—C(1)	−169.5 (0.5)	

* Isaac & Kennard (1972).

Table 4. *Puckering parameters (Cremer & Pople, 1975) for the pyranose and anhydride ring in 2,2′-di-O-acetyl-3,6;3′,6′-dianhydro-4,4′-dideoxy-α,α-trehalose*

The values in parentheses are those for the ring with the primed atoms.

	Pyranose ring		Anhydride ring	
q_2 (Å)	0.226	(0.244)	0.459	(0.465)
q_3 (Å)	−0.595	(−0.596)	–	
θ (°)	158.9	(158.3)	–	
φ (°)	65.2	(62.4)	78.5	(77.0)
Q (Å)	0.637	(0.660)	0.458	(0.469)

Computations were performed using the *SHELXTL-Plus* (Sheldrick, 1990) crystallographic software package.

the compound in solution so that it may not necessarily be the same as when in crystalline form. Nevertheless, the 3,6-anhydro derivatives of methyl-α-D-glucopyranoside and α,α-trehalose have been found to be devoid of sweetness (Lee & Birch, 1975) and this was suggested to be caused by strong intramolecular hydrogen bonding between the axial O(2) and O(4) OH groups as shown in the crystal structure of methyl-3,6-anhydro-α-D-glucopyranoside (Lindberg, Lindberg & Svensson, 1973). These OH groups are, therefore, not available for interaction with a complementary *A*H,*B* system of the taste receptor. Methyl-3,6-dianhydro-4-deoxy-α-D-*xylo*-hexopyranoside and the corresponding α,α-trehalose analogue are also devoid of sweet taste (Lee & Birch, 1975). Although the C(4) OH is absent in 3,6-dianhydro-4-deoxy-hexopyranoside structures, the X-ray data of (1) show that O(2) and O(2′) are ~3.0 Å from their respective ring O atoms, which is the optimum *A*-to-*B* distance for a sweet *A*H,*B* glucophore. However, O(2) and O(2′) are also ~2.6 Å from the anomeric O atom. In the unsubstituted derivative, it is, therefore, possible that OH(2) and OH(2′) form strong intramolecular hydrogen bonds to the anomeric O atom. The molecule will then have no *A*H,*B* glucophore and thus be devoid of sweet taste.

The γ function is viewed as a function that facilitates the accession of the molecule to a taste receptor and may be important for sweetness intensity. Although its role is generally agreed to be minimal, it is of structural interest to modify the γ effect. The removal of the C(4) OH group makes this position a potential γ site, but with the absence of an *A*H,*B* system this is mere speculation. This is presently being investigated.

Experimental

Crystal data

$C_{16}H_{22}O_9$
M_r = 358.3
Orthorhombic
$P2_12_12_1$
a = 8.231 (4) Å
b = 8.792 (5) Å
c = 23.60 (2) Å
V = 1708 (2) Å^3
Z = 4
D_x = 1.393 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 17 reflections
θ = 4.3–10.5°
μ = 0.115 mm^{-1}
T = 297 K
Prism
0.30 × 0.30 × 0.25 mm
Colourless
Crystal source: recrystallized from ethanol three times

Data collection

Siemens *R3m/V* diffractometer
ω scans
Absorption correction: none
1765 measured reflections
1765 independent reflections
1065 observed reflections [$F > 3.0\sigma(F)$]
θ_{max} = 25°
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 10$
$l = 0 \rightarrow 27$
2 standard reflections monitored every 98 reflections
intensity variation: ±1.5%

Refinement

Refinement on F
R = 0.0597
wR = 0.0537
S = 1.31
1065 reflections
227 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F) + 0.0005F^2]$
$(\Delta/\sigma)_{max}$ = 0.248
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: $F^* = F[1 + (0.002 \times \chi F^2/\sin 2\theta)]^{-1/4}$
Extinction coefficient: χ = 0.0008
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71584 (16 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HL1037]

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3,8α-Dihydroxyestra-1,3,5(10),6-tetraen-17-one

EDMUND W. CZERWINSKI*

Department of Human Biological Chemistry and Genetics, The University of Texas Medical Branch, Galveston, Texas 77555-0653, USA

ZHISONG CAO AND JOACHIM LIEHR

Department of Pharmacology, The University of Texas Medical Branch, Galveston, Texas 77555-0653, USA

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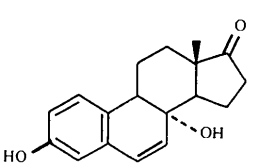
Abstract

The molecular parameters of the title compound, $C_{18}H_{20}O_3$, are all within normal limits. The *A*/*B* ring junction is planar and the *C*/*D* junction is *trans*, as expected. However, the *B*/*C* junction is *cis* with an interplanar angle of 65.1 (2)°. There are only two intermolecular contacts involving the 8α-hydroxyl of one molecule and the 3-hydroxyl and 17-keto O atoms on two symmetry related molecules.

Comment

The title compound (I) was synthesized as described by Cao & Liehr (1993). The crystal structure study was undertaken to ascertain the conformation of the compound and to determine on which face of the steroid skeleton the 8-hydroxyl group was located. Fig. 1 shows the structure of the molecule in the asymmetric unit with the thermal vibration ellipsoids of the non-H atoms. Bond lengths, bond angles and torsion angles of the non-H atoms are given in Table 2 and are within the range of expected values (Duax & Norton, 1975; Griffin, Duax & Weeks, 1984). The packing of the molecules is shown in Fig. 2. All intermolecular distances correspond to normal van der Waals interactions. The only intermolecular contacts involve O8 with O3($-x$, $y-\frac{1}{2}$, $\frac{1}{2}-z$) [2.715 (5) Å] and O17($\frac{1}{2}-x$, $2-y$, $z-\frac{1}{2}$) [2.804 (5) Å] resulting in an O3···O8···O17 angle of 92.3 (2)°. Steroid ring *A* (C1, C2, C3, C4, C5, C10) possesses bond parameters consistent with a benzene ring and is planar to within experimental error. The O3 hydroxyl group is coplanar with ring *A*. The asymmetry parameters defined by Duax & Norton (1975) for ring *A* range from 0.6 to 2.8° with $\langle\tau\rangle$ = 1.2°. Ring *B* (C5, C6, C7, C8, C9, C10) adopts a distorted sofa conformation largely due to the unsaturated C5—C10 and C6—C7 bonds. C9 is nearly coplanar with the plane formed by the atoms of ring *A* and O3. C7 and C8 deviate from this plane towards the α face of the molecule. The asymmetry parameters are $\Delta C_2^{5,6}$ = 7.2°, ΔC_s^6 = 14.9° and ΔC_s^7 = 39.9°, with $\langle\tau\rangle$ = 22.8°. These data indicate that ring *B* is distorted from the C9α,C10β-half-chair conformation (ΔC_2 = 0°) towards a C8α-sofa conformation. Ring *C* (C8, C9, C11, C12, C13, C14) does not have any unusual substituents and assumes the commonly found chair conformation ($\Delta C_2^{9,11}$ = 2.5°, ΔC_s^{11} = 3.0°, $\langle\tau\rangle$ = 55.4°).



(I)

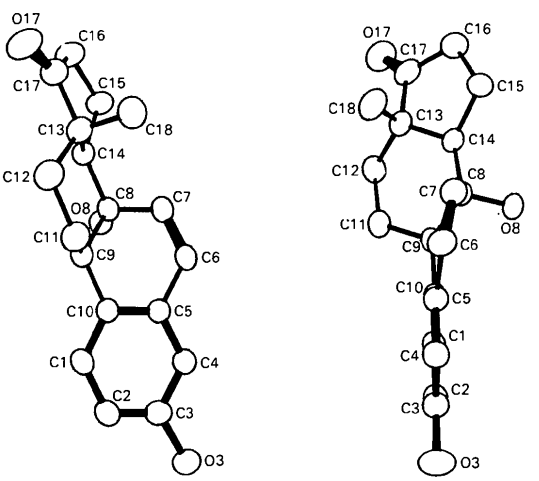


Fig. 1. Two orthogonal views of the molecular structure of the estratetraene in the asymmetric unit showing the numbering scheme and the thermal vibration ellipsoids of the non-H atoms. The thickest lines denote the double bonds.