used to refine structure: *SHELXL93*. Molecular graphics: *JACKAL* (Cockcroft, private program). Software used to prepare material for publication: *SHELXL93*.

Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: HU1101). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Cahill, P. A., Singer, K. D. & King, L. A. (1989). *Opt. Lett.* **14**, 1137–1139.

Metzger, R. M., Heimer, N. E. & Ashwell, G. J. (1984). *J. Mol. Cryst. Liq. Cryst.* **107**, 133–149.

Molecular Structure Corporation (1989). *TEXSAN. Single Crystal Structure Analysis*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Prasad, P. N. & Williams, D. J. (1991). *Introduction to Non-Linear Optical Effects in Molecules and Polymers*. New York: Wiley.

Sheldrick, G. M. (1985). *SHELXS86. Program for the Solution of Crystal Structures*. Univ. of Göttingen, Germany.

Sheldrick, G. M. (1993). *SHELXL93. Program for the Refinement of Crystal Structures*. Univ. of Göttingen, Germany.

Southgate, P. D. & Hall, D. S. (1971). *Appl. Phys. Lett.* **18**, 456–458.

Szablewski, M. (1994). *J. Org. Chem.* **59**, 954–956.

Taylor, R. & Kennard, O. (1982). *J. Am. Chem Soc.* **104**, 5063–5070.

Acta Cryst. (1995). C**51**, 718–721

(1R)-4,5-Benzocyclodeca-4-ene-2,6-diyn-1-yl 2,3,4,6-Tetra-O-acetyl-β-D-glucopyranoside and 4,5-Benzocyclodeca-4-ene-2,6-diyn-1-one

ALAIN COUSSON

Laboratoire Léon Brillouin (CEA-CNRS), CE Saclay, 91191 Gif sur Yvette CEDEX, France

ISABELLE DANCY AND JEAN-MARIE BEAU

Laboratoire de Biochimie Structurale, Université d'Orléans, BP 6759, 45067 Orléans CEDEX 2, France

(*Received* 21 *February* 1994; *accepted* 8 *July* 1994)

Abstract

The title compounds, $C_{28}H_{30}O_{10}$ and $C_{14}H_{10}O$, have been synthesized during the course of a program designed to prepare molecules with DNA-cleaving properties. The geometry of the strained benzodiyne system has been determined, the *S* configuration at the propargylic center established and the orientation of the sugar unit in relation to the aglycon defined. The results are compared with those for other derivatives. The molecular packing is governed by normal van der Waals interactions.

Comment

The glycosylated enediyne antibiotics such as calicheamicins and esperamicins have recently attracted a great deal of attention because of the potential antitumor properties of the enediyne moiety (Nicolaou & Dai, 1991; Lee, Ellestad & Borders, 1991). The carbohydrate domain is in part responsible for the sequence-selective double-stranded cleavage of various oligonucleotide targets by positioning the drug in the minor groove (Aiyar, Danishefsky & Crothers, 1992; Nicolaou, Tsay, Suzuki & Joyce, 1992). We undertook the preparation of simple models (Crévisy & Beau, 1991), including glycosylated congeners (I. Dancy & J.-M. Beau, unpublished results), compounds which may help to understand the mode-of-action of these substances.

Glucosylation of racemic benzodiynol (1) by the α-imidate (2) under the conditions of Schmidt (1986) provided the easily separated diastereomeric β-glucosides (3a) and (3b) according to the scheme below.

(1)   (2)   (3a)

(4)   (5)   (3b)

(I)
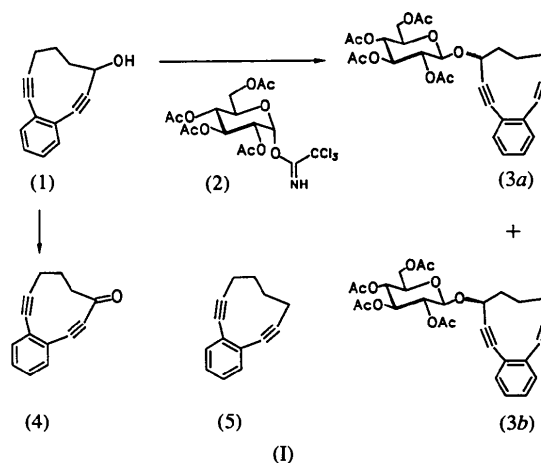
The structure of crystalline isomer (3a) was studied in order to establish the configuration at the propargylic center, to determine the structural parameters of the strained benzodiyne system and to define the orientation of the sugar unit in relation to the aglycon. The crystal structure of benzodiynone (4) is also reported for comparison.

The chemical reactivity of the ene(benzo)diyne systems can be correlated, to a first approximation, with the distance between the remote acetylenic C atoms, a measure of the molecular strain in the ground state

---

(Nicolaou & Dai, 1991). From this viewpoint, the most relevant structural parameters have been collated in Table 1 for the title compounds and for 3,4-benzocyclodeca-1,5-diyne (Bennett & Smith, 1977). From the values of the angles and transannular distances between the *sp* centers, it can be noted that substitution at a propargylic center [compare (3*a*) and (5)] or a change of geometry at C(1) [*sp*^{3} in (3*a*) and *sp*^{2} in (4)] does not significantly alter the strain in the ten-membered ring, which is mostly accommodated by the acetylenic centers. For the three compounds in Table 1 the distortion appears greatest at the acetylenic C atoms adjacent to the aromatic ring, in contrast to observations for ten-membered bicyclic conjugated ene–diyne systems (Schoenen, Porco, Schreiber, Van Duyne & Clardy, 1989).

The bridging unit C(1)—C(14)—C(13)—C(12) in compound (3*a*) is found in a chair-like conformation in which the propargylic O(1') atom lies in a
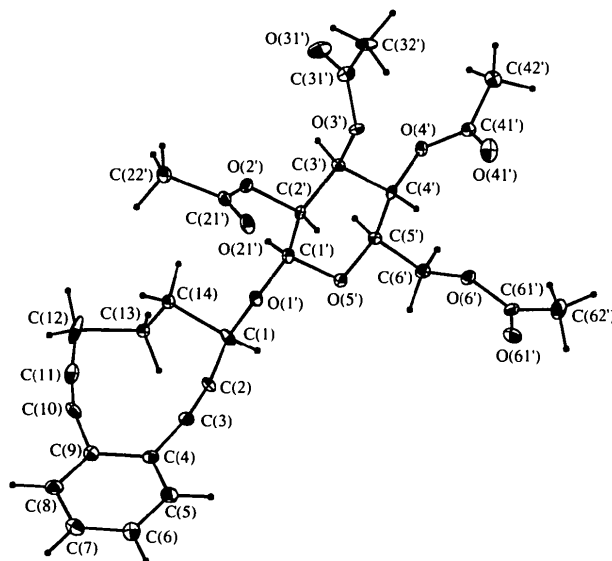
pseudo-equatorial position. The glycosidic torsion angles in (3*a*) are 79.85 (7)° [O(5')—C(1')—O(1')—C(1)] and −165.76 (6)° [C(1')—O(1')—C(1)—C(2)], and are within the normal ranges when compared with known conformations of β-D-glucopyranosyl derivatives in the solid state (Jeffrey & Sundaralingam, 1985).

Experimental

Compound (3*a*) was obtained by glucosylation of benzodiynol (1) using the α-trichloroacetimidate (2) in toluene at low temperature in the presence of trimethylsilyl trifluoromethanesulfonate, according to the procedure of Schmidt (1986). The two isomers (3*a*) and (3*b*) were separated by chromatography on silica gel and crystalline isomer (3*a*), $[\alpha]_D^{295K}$ = +70 (*c* 0.85 mg ml^{-1}, CHCl$_3$), was recrystallized from ethyl acetate; m.p. 427 K. Ketone (4) was obtained by oxidation of (1) and was recrystallized in hexane–ethyl ether; m.p. 377–378 K. Only very small crystals were obtained.

Fig. 1. *ORTEP* (Johnson, 1965) plot of molecule (3*a*). Displacement ellipsoids are drawn at the 30% probability level, except for those of C(13) and C(14) which are at an arbitrary level.
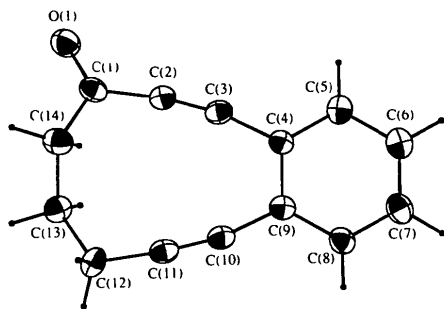

Fig. 2. *ORTEP* (Johnson, 1965) plot of molecule (4). Displacement ellipsoids are drawn at the 50% probability level.

Compound (3*a*)

Crystal data

C$_{28}$H$_{30}$O$_{10}$	Cu *K*α radiation
M_r = 526.538	λ = 1.5418 Å
Orthorhombic	Cell parameters from 25
$P2_12_12_1$	reflections
a = 31.10 (1) Å	θ = 17.5–20.25°
b = 9.452 (5) Å	μ = 0.759 mm^{-1}
c = 9.507 (4) Å	T = 293 K
V = 2795 (2) Å^3	Thin plate
Z = 4	0.2 × 0.15 × 0.01 mm
D_x = 1.251 Mg m^{-3}	Colourless

Data collection

Philips PW1100 diffractometer	θ_{max} = 67°
	h = 0 → 34
ω–2θ scans	k = 0 → 10
Absorption correction:	l = 0 → 10
refined from ΔF	3 standard reflections
T_{min} = 0.73, T_{max} = 1.00	frequency: 60 min
2400 measured reflections	intensity decay:
2400 independent reflections	<0.02%
1424 observed reflections	
[$I \geq 3\sigma(I)$]	

Refinement

Refinement on F	$(\Delta/\sigma)_{max}$ = 0.3
R = 0.065	$\Delta\rho_{max}$ = 0.31 e Å^{-3}
wR = 0.078	$\Delta\rho_{min}$ = −0.36 e Å^{-3}
S = 1.05	Extinction correction:
1424 reflections	Larson (1970)
345 parameters	Extinction coefficient:
One common U refined for all H atoms	36 (20)
Weighting scheme:	Atomic scattering factors
Chebychev polynomial	from *International Tables*
with parameters 10.4,	*for X-ray Crystallography*
0.676, 8.55	(1974, Vol. IV)

Table 1. Comparison of selected bond angles (°), cisoid deformations (°) and transannular distances (Å) in the ten-membered rings in compounds (3a), (4) and (5)^a

	(3a)	(4)	(5)
Angle			
C(1)—C(2)—C(3)	169.1 (8)	169.4 (2)	174.8
C(2)—C(3)—C(4)	168.3 (8)	168.9 (2)	166.7
C(9)—C(10)—C(11)	165.5 (9)	166.3 (2)	–
C(10)—C(11)—C(12)	173.2 (10)	172.6 (2)	–
Cisoid deformation			
C(2)	10.9	10.6	5.2
C(3)	11.7	11.1	13.3
C(10)	14.5	13.7	–
C(11)	6.8	7.4	–
Transannular distance			
C(2)···C(11)	3.338 (12)	3.325 (2)	3.261
C(3)···C(10)	2.732 (11)	2.711 (2)	2.806

Reference: (a) Bennett & Smith (1977).

Table 2. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (3a)

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

	x	y	z	U$_{eq}$
O(1')	0.1455 (1)	0.6963 (6)	0.4667 (5)	0.0636
O(2')	0.1413 (1)	0.4035 (6)	0.4460 (6)	0.0685
O(3')	0.2238 (2)	0.2700 (5)	0.5025 (5)	0.0577
O(4')	0.2908 (1)	0.4034 (5)	0.3407 (4)	0.0547
O(5')	0.2176 (1)	0.6927 (5)	0.4193 (5)	0.0607
O(6')	0.3133 (2)	0.7021 (6)	0.4784 (5)	0.0718
O(21')	0.1210 (2)	0.4202 (8)	0.6713 (7)	0.0935
O(31')	0.2119 (3)	0.1177 (8)	0.3300 (7)	0.1107
O(41')	0.3266 (2)	0.3535 (9)	0.5362 (6)	0.0946
O(61')	0.3532 (2)	0.8885 (9)	0.422 (1)	0.1186
C(1')	0.1778 (2)	0.6188 (9)	0.3999 (7)	0.0597
C(2')	0.1807 (2)	0.4801 (8)	0.4739 (7)	0.0524
C(3')	0.2174 (2)	0.3928 (7)	0.4162 (7)	0.0550
C(4')	0.2588 (2)	0.4788 (7)	0.4167 (7)	0.0458
C(5')	0.2518 (2)	0.6208 (8)	0.3476 (7)	0.0516
C(6')	0.2907 (3)	0.721 (1)	0.3470 (8)	0.0722
C(21')	0.1134 (2)	0.392 (1)	0.552 (1)	0.0764
C(22')	0.0711 (3)	0.331 (1)	0.496 (1)	0.0948
C(31')	0.2208 (3)	0.1426 (9)	0.4493 (9)	0.0786
C(32')	0.2272 (4)	0.0289 (9)	0.557 (1)	0.0930
C(41')	0.3221 (3)	0.3395 (9)	0.4129 (8)	0.0680
C(42')	0.3504 (3)	0.2520 (9)	0.3219 (9)	0.0745
C(61')	0.3460 (3)	0.792 (1)	0.498 (1)	0.0833
C(62')	0.3723 (4)	0.755 (2)	0.620 (1)	0.1199
C(1)	0.1290 (3)	0.8169 (9)	0.3911 (8)	0.0649
C(2)	0.1051 (2)	0.8966 (9)	0.4954 (8)	0.0668
C(3)	0.0796 (2)	0.9496 (8)	0.5735 (9)	0.0701
C(4)	0.0430 (2)	1.0113 (8)	0.6435 (8)	0.0706
C(5)	0.0456 (3)	1.065 (1)	0.7787 (9)	0.0915
C(6)	0.0096 (3)	1.125 (1)	0.840 (1)	0.1067
C(7)	−0.0293 (3)	1.121 (1)	0.771 (1)	0.0971
C(8)	−0.0326 (3)	1.064 (1)	0.637 (1)	0.0924
C(9)	0.0038 (2)	1.0093 (8)	0.5730 (9)	0.0714
C(10)	0.0025 (3)	0.946 (1)	0.436 (1)	0.0830
C(11)	0.0109 (3)	0.894 (1)	0.327 (1)	0.1000
C(12)	0.0263 (4)	0.824 (2)	0.199 (1)	0.1351
C(13)	0.0744 (6)	0.847 (3)	0.190 (2)	0.2408
C(14)	0.0956 (5)	0.756 (2)	0.275 (1)	0.1069

Table 3. Selected geometric parameters (Å, °) for (3a)

O(1')—C(1')	1.397 (8)	C(5')—C(6')	1.54 (1)
O(1')—C(1)	1.442 (9)	C(21')—C(22')	1.53 (1)
O(2')—C(2')	1.450 (8)	C(31')—C(32')	1.50 (1)

O(2')—C(21')	1.33 (1)	C(41')—C(42')	1.49 (1)
O(3')—C(3')	1.436 (8)	C(61')—C(62')	1.46 (2)
O(3')—C(31')	1.31 (1)	C(1)—C(2)	1.45 (1)
O(4')—C(4')	1.421 (7)	C(1)—C(14)	1.62 (2)
O(4')—C(41')	1.336 (8)	C(2)—C(3)	1.196 (9)
O(5')—C(1')	1.431 (8)	C(3)—C(4)	1.44 (1)
O(5')—C(5')	1.435 (8)	C(4)—C(5)	1.384 (8)
O(6')—C(6')	1.44 (1)	C(4)—C(9)	1.392 (7)
O(6')—C(61')	1.34 (1)	C(5)—C(6)	1.385 (8)
O(21')—C(21')	1.19 (1)	C(6)—C(7)	1.380 (8)
O(31')—C(31')	1.19 (1)	C(7)—C(8)	1.382 (8)
O(41')—C(41')	1.187 (8)	C(8)—C(9)	1.386 (8)
O(61')—C(61')	1.19 (1)	C(10)—C(11)	1.18 (1)
C(1')—C(2')	1.49 (1)	C(10)—C(9)	1.44 (1)
C(2')—C(3')	1.511 (9)	C(11)—C(12)	1.46 (1)
C(3')—C(4')	1.524 (9)	C(12)—C(13)	1.51 (2)
C(4')—C(5')	1.51 (1)	C(13)—C(14)	1.35 (2)
C(1')—O(1')—C(1)	116.4 (5)	O(31')—C(31')—C(32')	122.8 (8)
C(2')—O(2')—C(21')	117.0 (6)	O(4')—C(41')—O(41')	122.9 (8)
C(3')—O(3')—C(31')	120.8 (5)	O(4')—C(41')—C(42')	112.6 (6)
C(4')—O(4')—C(41')	118.3 (5)	O(41')—C(41')—C(42')	124.5 (8)
C(1')—O(5')—C(5')	110.4 (5)	O(6')—C(61')—O(61')	122.9 (9)
C(6')—O(6')—C(61')	114.5 (7)	O(6')—C(61')—C(62')	112.8 (9)
O(1')—C(1')—O(5')	107.9 (6)	O(61')—C(61')—C(62')	124.3 (9)
O(1')—C(1')—C(2')	106.9 (5)	O(1')—C(1)—C(2)	104.6 (6)
O(5')—C(1')—C(2')	108.5 (5)	O(1')—C(1)—C(14)	106.7 (8)
O(2')—C(2')—C(1')	107.6 (5)	C(2)—C(1)—C(14)	108.5 (7)
O(2')—C(2')—C(3')	107.4 (5)	C(1)—C(2)—C(3)	169.1 (8)
C(1')—C(2')—C(3')	110.8 (6)	C(2)—C(3)—C(4)	168.3 (8)
O(3')—C(3')—C(2')	109.8 (5)	C(3)—C(4)—C(5)	122.1 (7)
O(3')—C(3')—C(4')	108.2 (5)	C(3)—C(4)—C(9)	117.6 (7)
C(2')—C(3')—C(4')	110.2 (5)	C(5)—C(4)—C(9)	120.2 (7)
O(4')—C(4')—C(3')	108.8 (5)	C(4)—C(5)—C(6)	119.8 (9)
O(4')—C(4')—C(5')	109.0 (5)	C(5)—C(6)—C(7)	119.6 (9)
C(3')—C(4')—C(5')	110.5 (5)	C(6)—C(7)—C(8)	121.1 (9)
O(5')—C(5')—C(4')	108.8 (5)	C(7)—C(8)—C(9)	119.3 (9)
O(5')—C(5')—C(6')	107.2 (6)	C(10)—C(9)—C(4)	117.9 (7)
C(4')—C(5')—C(6')	115.7 (6)	C(10)—C(9)—C(8)	122.2 (8)
O(6')—C(6')—C(5')	107.8 (6)	C(4)—C(9)—C(8)	119.9 (8)
O(2')—C(21')—O(21')	125.0 (7)	C(11)—C(10)—C(9)	165.5 (9)
O(2')—C(21')—C(22')	109.0 (8)	C(10)—C(11)—C(12)	173.2 (10)
O(21')—C(21')—C(22')	126.0 (8)	C(11)—C(12)—C(13)	108.0 (12)
O(3')—C(31')—O(31')	124.5 (9)	C(12)—C(13)—C(14)	111.0 (19)
O(3')—C(31')—C(32')	112.6 (7)	C(1)—C(14)—C(13)	119.9 (17)

Compound (4)

Crystal data

Data collection

Refinement

Refinement on F	$(\Delta/\sigma)_{max} = 0.06$
$R = 0.048$	$\Delta\rho_{max} = 0.13$ e Å^{-3}
$wR = 0.028$	$\Delta\rho_{min} = -0.14$ e Å^{-3}
$S = 1.12$	Extinction correction:
1220 reflections	Larson (1970)
138 parameters	Extinction coefficient:
One common U refined for	57 (11)
all H atoms	Atomic scattering factors
Weighting scheme:	from *International Tables*
Chebychev polynomial	*for X-ray Crystallography*
with parameters 22.8,	(1974, Vol. IV)
−48.8, 21.3 and −18.2	

Table 4. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (4)*

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

	x	y	z	U_{eq}
C(1)	0.69460 (9)	1.0319 (1)	0.0562 (2)	0.0673
C(2)	0.6295 (1)	1.0143 (1)	0.1365 (2)	0.0694
C(3)	0.57191 (9)	0.9888 (1)	0.1853 (2)	0.0631
C(4)	0.50504 (8)	0.9396 (1)	0.2270 (2)	0.0595
C(5)	0.4618 (1)	0.9833 (2)	0.3341 (2)	0.0689
C(6)	0.3994 (1)	0.9274 (2)	0.3739 (2)	0.0763
C(7)	0.3803 (1)	0.8286 (2)	0.3064 (2)	0.0779
C(8)	0.4215 (1)	0.7858 (1)	0.1976 (2)	0.0716
C(9)	0.48462 (9)	0.8396 (1)	0.1569 (2)	0.0616
C(10)	0.53220 (9)	0.7977 (1)	0.0488 (2)	0.0651
C(11)	0.5812 (1)	0.7790 (1)	−0.0298 (2)	0.0675
C(12)	0.6471 (1)	0.7648 (2)	−0.1136 (2)	0.0770
C(13)	0.7092 (1)	0.8360 (2)	−0.0540 (2)	0.0736
C(14)	0.7015 (1)	0.9634 (2)	−0.0765 (2)	0.0790
O(1)	0.74006 (8)	1.0993 (1)	0.0929 (2)	0.0882

Table 5. *Selected geometric parameters (Å, °) for (4)*

C(1)—C(2)	1.440 (3)	C(6)—C(7)	1.381 (3)
C(1)—C(14)	1.495 (3)	C(7)—C(8)	1.373 (3)
C(1)—O(1)	1.213 (2)	C(8)—C(9)	1.388 (3)
C(2)—C(3)	1.200 (3)	C(9)—C(10)	1.432 (3)
C(3)—C(4)	1.427 (2)	C(10)—C(11)	1.195 (2)
C(4)—C(5)	1.387 (2)	C(11)—C(12)	1.463 (3)
C(4)—C(9)	1.411 (2)	C(12)—C(13)	1.535 (3)
C(5)—C(6)	1.385 (3)	C(13)—C(14)	1.535 (3)
C(2)—C(1)—C(14)	115.4 (2)	C(6)—C(7)—C(8)	120.9 (2)
C(2)—C(1)—O(1)	122.0 (2)	C(7)—C(8)—C(9)	120.3 (2)
C(14)—C(1)—O(1)	122.5 (2)	C(4)—C(9)—C(8)	119.1 (2)
C(1)—C(2)—C(3)	169.4 (2)	C(4)—C(9)—C(10)	117.3 (1)
C(2)—C(3)—C(4)	168.9 (2)	C(8)—C(9)—C(10)	123.6 (2)
C(3)—C(4)—C(5)	123.2 (2)	C(9)—C(10)—C(11)	166.3 (2)
C(3)—C(4)—C(9)	116.8 (2)	C(10)—C(11)—C(12)	172.6 (2)
C(5)—C(4)—C(9)	119.9 (2)	C(11)—C(12)—C(13)	111.5 (1)
C(4)—C(5)—C(6)	119.9 (2)	C(12)—C(13)—C(14)	115.0 (2)
C(5)—C(6)—C(7)	119.9 (2)	C(1)—C(14)—C(13)	115.5 (1)

The structures were solved using direct methods and successive Fourier maps (*SHELXS*86; Sheldrick, 1985) and refined using *CRYSTALS* (Watkin, Carruthers & Betteridge, 1985). Figures were drawn using *ORTEP* (Johnson, 1965). H-atom positions were calculated. In compound (3a), large displacement parameters were found for C(12), C(13) and C(14) with large standard deviations on the positional parameters. Restraints on bonds and angles were used in the refinement to obtain this part of the structure and successive refinement steps did not affect the rest of the structure. There was no evidence for disorder such as that found by Bennett & Smith (1977) for 3,4-benzocyclodeca-1,5-diyne. The slightly high R value for (3a) is due to the small size of the sample and the low ratio of observations to parameters.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and bond distances and angles involving H atoms, along with stereoviews of the crystal packing have been deposited with the IUCr (Reference: PA1115). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Aiyar, J., Danishefsky, S. J. & Crothers, D. M. (1992). *J. Am. Chem. Soc.* **114**, 7552–7554.
Bennett, M. J. & Smith, R. A. (1977). *Acta Cryst.* B33, 1123–1126.
Crévisy, C. & Beau, J. M. (1991). *Tetrahedron Lett.* 32, 3171–3174.
Jeffrey, G. A. & Sundaralingam, M. (1985). *Adv. Carbohydr. Chem. Biochem.* 43, 203–421.
Johnson, C. K. (1965). *ORTEP.* Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.
Larson, A. C. (1970). *Crystallographic Computing,* edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 291–294. Copenhagen: Munksgaard.
Lee, M. D., Ellestad, G. A. & Borders, D. B. (1991). *Acc. Chem. Res.* **24**, 235–243.
Nicolaou, K. C. & Dai, W. M. (1991). *Angew. Chem. Int. Ed. Engl.* **30**, 1387–1530.
Nicolaou, K. C., Tsay, S. C., Suzuki, T. & Joyce, G. F. (1992). *J. Am. Chem. Soc.* **114**, 7555–7557.
Schmidt, R. R. (1985). *Angew. Chem. Int. Ed. Engl.* **25**, 212–235.
Sheldrick, G. M. (1985). *SHELXS86. Program for the Solution of Crystal Structures.* Univ. of Göttingen, Germany.
Schoenen, F. J., Porco, J. A., Schreiber, S. L., Van Duyne, G. D. & Clardy, J. (1989). *Tetrahedron Lett.* 29, 3765–3768.
Watkin, D. J., Carruthers, J. R. & Betteridge, P. W. (1985). *CRYSTALS User Guide.* Chemical Crystallography Laboratory, Univ. of Oxford, England.

3'-Methoxyspiro[bicyclo[3.1.0]hexane-6,16'-estra-1',3',5'(10')-trien]-17'-one

Rob W. W. Hooft

EMBL, Meyerhofstrasse 1, D-69117 Heidelberg, Germany

Jan Kroon

Bijvoet Center for Biomolecular Research, Department of Crystal and Structural Chemistry, Utrecht University, Padualaan 8, 3584 CH Utrecht, The Netherlands

Abstract

The title compound, $C_{24}H_{30}O_2$, is a substituted steroid structure. Ring A is planar, ring B adopts a distorted half-chair conformation, ring C a chair conformation,