2·849 (2) Å. The O(2), C(11), C(8), C(7), N(1), H(N1) moiety is planar within 0·03 Å and the O(3), C(9), C(8), C(11), N(2), H(N2) moiety is planar within 0·01 Å. There is no evidence of intermolecular hydrogen bonding.

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Synthesis of Cedranoid Sesquiterpenes. IV. X-ray Characterization of the endo-6-Hydroxy-endo-8-methyl and exo-6-Hydroxy-exo-8-methyl Isomers of Methyl 6-Hydroxy-4,4,8-trimethyl-3-oxo-cis-bicyclo[3.3.0]octane-1-carboxylate

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Abstract. $C_{13}H_{20}O_4$, endo-endo isomer (1), $M_r = 240·3$, monoclinic, $P2/n$, $a = 15·041$ (3), $b = 6·225$ (3), $c = 27·795$ (5) Å, $\beta = 101·56$ (2)°, $U = 2550$ (2) Å^3, $Z = 8$ (2 independent molecules), $D_x = 1·25$ g cm^{-3}, Mo $K\bar{\alpha}$ radiation, $\lambda = 0·71069$ Å, $\mu = 0·9$ cm^{-1}, $F(000) = 1040$, $T = 298$ K, $R = 0·090$, $wR = 0·071$ for 1499 reflections with $I \geq 2\sigma(I)$. exo-exo Isomer (2), $M_r = 240·3$, rhombohedral, $R\bar{3}$, $a = 12·916$ (7) Å, $\alpha = 92·86$ (5)°, $U = 2146$ (4) Å^3, $Z = 6$, $D_x = 1·12$ g cm^{-3}, Mo $K\bar{\alpha}$ radiation, $\mu = 0·8$ cm^{-1}, $F(000) = 780$, $T = 298$ K, $R = 0·062$, $wR = 0·064$ for 1306 reflections with $I \geq 3\sigma(I)$. In isomer (1), the two independent molecules in the asymmetric unit are approximate mirror images and the 6-hydroxy and 8-methyl substituents are both endo. The cyclopentane rings are both flattened envelopes and there are significant transannular O=C···OH contacts (2·88 and 2·91 Å) in both molecules. In isomer (2), the C(6) and C(8) substituents are both exo and the cyclopentane rings have distorted envelope and half-chair conformations. The molecules of this isomer are linked by hydrogen bonding into hexameric units.

configurations in two such intermediates, (1) and (2), by X-ray crystallography.

(1)   (2)   (3)   (4)

(E = CO$_2$Me)

Introduction. Synthetic routes to the cedranoid sesquiterpenes being pursued in these laboratories (Yates, Burnell, Freer & Sawyer, 1987; Grewal, Hayes, Sawyer & Yates, 1987) have involved the preparation of several bicyclo[3.3.0]octanes as intermediates. In this paper we report on the determination of the relative
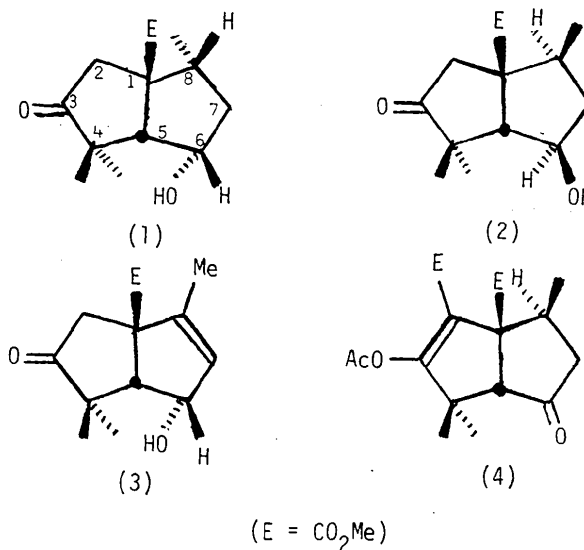
Experimental. Isomer (1) was prepared by hydrogenation of (3), as described elsewhere (Yates, Burnell, Freer & Sawyer, 1987). Crystallization from pentane containing 5–10% dichloromethane gave colorless crystals as small thin needles, m.p. 395·6–396·1 K. Crystal of overall dimensions 0·019 × 0·069 ×

Table 1. *Experimental details*

	Isomer (1)	Isomer (2)
Reflections for cell determination*	25/	25/
|Number/2θ range (°)|	7·2 < 2θ < 27·8	19·9 < 2θ < 28·8
ω scan range (°)	0·75 + 0·35tanθ	0·85 + 0·35tanθ
Max. time in final scan (s)†	70	65
Standard reflections |Number/interval (s)|	3/8500‡	3/8000§
Max. 2θ(°)/octants	50/$h,k,\pm l$	50/$h,\pm k,\pm l$
Number of data collected (including standards)	4814	7413
	(h_{max}=13, k_{max}=6, l_{max}=32)	(h_{max}=11, k_{max}=10, l_{max}=15)
Structure solution	Direct methods (*MULTAN*11/82)	Direct methods (*SHELX*76)
Number of data in least squares	1499 |$I \geq 2\sigma(I)$|	1306 |$I \geq 3\sigma(I)$|¶
Final R (wR)	0·0897 (0·0705)	0·0620 (0·0639)
Max. Δ/σ in final cycle	0·60**	0·25**
Factor used in weighting scheme††	0·00022	0·00060
Max. $\Delta\rho$ (e Å^{-1})	<0·16	0·41

* Enraf–Nonius CAD-4 diffractometer; graphite-monochromatized Mo $K\bar{\alpha}$ radiation; ω–2θ scans; $T = 298$ K. Lorentz and polarization corrections applied to all data collected.

† Scan rates conditional on information collected in prescans were selected to give $I/\sigma(I) > 25$ within max. scan time specified. Backgrounds by extending scan by 25% on either side of peak measured for half the time taken to collect the peak.

‡ No significant variations with time observed.

§ ca 7% losses in intensities corrected for at data reduction (max. rescale factor = 1·127).

¶ Zero F_o's rejected and 3588 symmetry-equivalent data averaged ($R_{merge} = 0·041$) to give 2415 unique reflections.

** Maximum shifts for methyl rigid groups.

†† $w = [\sigma^2(F) + pF^2]^{-1}$.

0·350 mm used throughout. Isomer (2) was prepared by reduction of the ketonic group of (4) with sodium borohydride followed by hydrolysis and monodecarbomethoxylation (Grewal, Hayes, Sawyer & Yates, 1987). Crystallization from ethyl acetate/hexane gave colorless rhombs, m.p. 333·6–337·1 K. Crystal of overall dimensions 0·225 × 0·250 × 0·275 mm used throughout. Precession photographs to check crystal quality. Further work on the diffractometer gave the experimental results summarized in Table 1. For isomer (1) the small size of the crystal limited the number of observed data available even when the criterion $I \geq 2\sigma(I)$ was used, leading to high R values. Similarly, peaks from crystal of isomer (2) were somewhat broad (scan widths of reflections used in cell determination were 1·11–1·60°) and a large number of extra symmetry-related data were eventually collected and averaged to improve the quality of the data set (see Table 1 for details). Both structures were solved by direct methods and refined by least-squares and Fourier methods. H atoms were first located in ΔF maps before the positions of the CH, CH$_2$ and CH$_3$ H atoms were optimized. For isomer (1), the positions of the hydroxyl H atoms were fixed at their positions in a ΔF map, while in isomer (2), the positional parameters of the hydroxyl H atom were allowed to refine. In both isomers, methyl groups were refined as rigid groups. Least-squares refinement minimizing $\sum w\Delta F^2$ [all non-H atoms anisotropic, 2 blocks for isomer (1)] converged to the indicated agreement indices. Two residual peaks in isomer (2) of heights 0·4 and 0·3 e Å^{-3} were on special positions. Refinement of the occupancies of these peaks with U fixed at 0·15 Å^2 indicated at most 10% of a C

Table 2. *Final atomic positional and thermal parameters* ($\text{Å}^2 \times 10^3$)

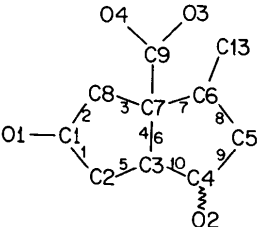First line is molecule 1, second is molecule 2 in isomer (1) and third line is isomer (2)

$$U_{eq} = \tfrac{1}{3}\text{trace } \mathbf{U}.$$

	x	y	z	U_{eq}
O(1)	0·6478 (5)	−0·2874 (10)	−0·1208 (2)	59 (5)
	0·5653 (4)	1·0355 (10)	0·6586 (2)	58 (5)
	0·4928 (2)	−0·1275 (3)	−0·0486 (2)	90 (2)
O(2)	0·8546 (4)	−0·0040 (11)	−0·0765 (2)	51 (5)
	0·5865 (4)	0·7419 (11)	0·7726 (2)	47 (4)
	0·8458 (2)	0·0169 (2)	0·1309 (2)	64 (2)
O(3)	0·6406 (4)	0·2883 (11)	0·0233 (2)	44 (5)
	0·3147 (5)	0·3984 (11)	0·6729 (2)	54 (5)
	0·6870 (3)	−0·1988 (3)	0·3391 (3)	103 (3)
O(4)	0·6126 (4)	−0·0561 (11)	0·0367 (2)	56 (5)
	0·2790 (5)	0·7204 (11)	0·6414 (2)	59 (5)
	0·5218 (3)	−0·2428 (4)	0·3040 (4)	146 (4)
C(1)	0·6693 (7)	−0·1477 (16)	−0·0901 (3)	40 (7)
	0·5242 (6)	0·8843 (16)	0·6720 (3)	31 (6)
	0·5449 (3)	−0·1311 (3)	0·0309 (3)	64 (3)
C(2)	0·6611 (7)	0·0912 (15)	−0·0999 (3)	37 (7)
	0·5498 (6)	0·6482 (14)	0·6686 (3)	28 (6)
	0·6601 (3)	−0·1523 (3)	0·0388 (3)	61 (3)
C(3)	0·7260 (6)	0·1857 (14)	−0·0554 (3)	29 (6)
	0·4975 (5)	0·5450 (14)	0·7052 (3)	27 (6)
	0·6965 (3)	−0·1037 (3)	0·1460 (3)	53 (2)
C(4)	0·8256 (7)	0·1976 (16)	−0·0580 (3)	41 (7)
	0·5446 (6)	0·5353 (16)	0·7587 (3)	43 (7)
	0·7383 (3)	0·0086 (3)	0·1529 (3)	49 (2)
C(5)	0·8716 (6)	0·2171 (16)	−0·0050 (3)	48 (7)
	0·4674 (6)	0·5037 (17)	0·7859 (3)	51 (7)
	0·7189 (3)	0·0454 (3)	0·2625 (3)	64 (3)
C(6)	0·8191 (6)	0·0673 (14)	0·0242 (3)	32 (6)
	0·3901 (6)	0·6488 (15)	0·7586 (3)	37 (6)
	0·6078 (3)	0·0049 (3)	0·2740 (3)	65 (3)
C(7)	0·7250 (6)	0·0317 (15)	−0·0111 (3)	32 (6)
	0·4131 (6)	0·6823 (15)	0·7059 (3)	32 (6)
	0·5992 (3)	−0·1036 (3)	0·2140 (3)	59 (2)
C(8)	0·7066 (6)	−0·1920 (14)	−0·0366 (3)	28 (6)
	0·4409 (6)	0·9103 (15)	0·6925 (3)	41 (7)
	0·5043 (3)	−0·1161 (4)	0·1377 (3)	74 (3)
C(9)	0·6527 (6)	0·0763 (18)	0·0170 (3)	34 (7)
	0·3295 (7)	0·6100 (17)	0·6700 (4)	40 (8)
	0·5968 (4)	−0·1909 (4)	0·2882 (4)	88 (3)
C(10)	0·5761 (6)	0·3455 (16)	0·0533 (3)	52 (7)
	0·2335 (6)	0·3090 (18)	0·6430 (4)	65 (8)
	0·6892 (6)	−0·2738 (7)	0·4178 (6)	169 (7)
C(11)	0·5613 (6)	0·1512 (16)	−0·0977 (3)	47 (7)
	0·5067 (6)	0·5782 (14)	0·6161 (3)	40 (6)
	0·6658 (4)	0·2714 (3)	0·0378 (4)	95 (4)
C(12)	0·6795 (6)	0·1553 (15)	−0·1505 (3)	41 (6)
	0·6517 (6)	0·6094 (16)	0·6782 (3)	49 (7)
	0·7170 (4)	−0·1116 (4)	−0·0516 (3)	83 (3)
C(13)	0·8743 (6)	−0·1374 (16)	0·0413 (3)	53 (8)
	0·3823 (7)	0·8584 (16)	0·7869 (3)	62 (8)
	0·5741 (4)	0·0082 (5)	0·3863 (3)	100 (4)

atom and these peaks were excluded from the final refinements. Calculations were on PDP 11/23 and Gould 9705 computers using programs in the *SHELX* (Sheldrick, 1976), *MULTAN* (Main *et al.*, 1982) and Enraf–Nonius *SDP* packages (Frenz, 1981). Scattering factors stored in the programs were taken from *International Tables for X-ray Crystallography* (1974).

The final atomic positional parameters, selected torsion angles, bond lengths and bond angles for both isomers and details of the hydrogen bonding in isomer (2) are given in Tables 2–5, respectively.*

* Lists of structure-factor amplitudes, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44392 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 3. *Selected torsion angles* (°) *and puckering constants* (°) *for the cyclopentane rings*

Torsion angle	Isomer (1)		Isomer (2)
	Molecule 1	Molecule 2	
1	19·9 (7) ⎫	−19·5 (7) ⎫	−23·9 (3) ⎫
2	−1·0 (7) ⎪ Δ = 32 (4)*	2·9 (8) ⎪ Δ = 26 (4)	12·5 (3) ⎪ Δ = 19 (2)
3	−17·9 (7) ⎬ φ_m = −33 (1)	15·3 (7) ⎬ φ_m = 30 (1)	4·1 (3) ⎬ φ_m = 26·1 (4)
4	30·9 (7) ⎪	−28·2 (7) ⎪	−18·9 (3) ⎪
5	−31·4 (7) ⎭	29·0 (7) ⎭	25·7 (3) ⎭
6	30·0 (7) ⎫	−27·3 (7) ⎫	−12·2 (3) ⎫
7	−6·6 (7) ⎪ Δ = 19 (3)	3·4 (7) ⎪ Δ = 26 (3)	−15·5 (3) ⎪ Δ = 4 (1)
8	−19·6 (7) ⎬ φ_m = −43 (1)	21·7 (7) ⎬ φ_m = 43 (1)	37·7 (3) ⎬ φ_m = −46·0 (3)
9	38·8 (7) ⎪	−39·5 (7) ⎪	−46·0 (3) ⎪
10	−42·4 (7) ⎭	41·4 (7) ⎭	35·9 (3) ⎭
C(3)—C(7)—C(9)—O(3)	−40·6 (9)	49·1 (9)	47·0 (4)
C(3)—C(7)—C(9)—O(4)	145·9 (9)	−131·5 (10)	−137·1 (5)
C(13)—C(6)—C(7)—C(3)	−129·0 (6)	125·9 (6)	−142·9 (3)
C(13)—C(6)—C(7)—C(8)	−16·0 (8)	10·1 (8)	102·6 (4)
C(13)—C(6)—C(7)—C(9)	107·9 (7)	−113·0 (7)	−21·0 (4)
O(2)—C(4)—C(3)—C(2)	−45·6 (8)	45·2 (8)	−84·1 (3)
O(2)—C(4)—C(3)—C(7)	72·2 (7)	−73·8 (7)	157·4 (3)
C(2)—C(3)—C(7)—C(6)	154·4 (6)	−152·7 (6)	−137·9 (3)
C(4)—C(3)—C(7)—C(8)	−93·5 (6)	97·2 (7)	106·8 (3)
Fold angle, θ†	124·0 (6)	125·0 (7)	122·4 (3)

* Altona, Geise & Romers (1968).

† θ is defined as $\frac{1}{2}$|| τ[C(2)—C(3)—C(7)—C(6)]| + |τ[C(4)—C(3)—C(7)—C(8)]||.

Discussion.* The two independent molecules in the asymmetric unit of isomer (1) both have the hydroxyl and secondary methyl substituents *endo* and are approximate mirror images (Figs. 1 and 2). Thus, a best molecular fit of the mirror image of molecule 2 to molecule 1 using the program *BMFIT* (Yuen & Nyburg, 1979) shows that atoms C(1) to C(8) in the two molecules fit to within 0·05 Å, while the deviations of the other non-H atoms are (in Å): O(1), 0·058; O(2), 0·054; O(3), 0·317; O(4), 0·241; C(9), 0·095; C(10), 0·439; C(11), 0·059; C(12), 0·068 and C(13), 0·144. The maximum deviations are for the methoxycarbonyl groups, which are slightly rotated with respect to each other {Δτ[C(3)—C(7)—C(9)—O(4)] = 14 (2); Δτ[C(3)—C(7)—C(9)—O(3)] = 9 (2)°, Table 3}. In the asymmetric unit the angular difference between the vectors C(1)→C(5) and C(3)→C(7) defining the length and width of the two molecules is 97 and 101°, respectively.

Selected torsion angles in Table 3 indicate that the conformations of the cyclopentane rings in both molecules of isomer (1) are non-ideal but have puckering constants slightly closer to those expected for envelope (C_s; Δ = 36°, φ_m = 46·7°) rather than for half-chair (C_2; Δ = 0°, φ_m = 46·7°) conformations. The crystal packing of this isomer consists of layers of

molecules approximately in the (10Ī) plane (Fig. 2). There is a hydrogen bond [O(2)_{mol 1}···O(1)_{mol 2} ($\frac{3}{2}$−x, −1+y, −$\frac{1}{2}$−z) = 2·80 Å; H(1)_{mol 1}···O(1)_{mol 2} = 1·68 Å] between the molecules. Other intermolecular contacts are generally weak. Both molecules, however, contain intramolecular O(2)···C(1) contacts [2·88 and 2·91 (1) Å], which have been considered to be of some significance in other bicyclo[3.3.0]octane and related structures (Burgi, Dunitz & Shefter, 1974; Murray-Rust, Glen, Newton & Ali, 1982). The strongest of these interactions are *ca* 2·6 Å in length and at distances > 3·1 Å are generally negligible.

In isomer (2), both the hydroxyl and the secondary methyl substituents are *exo* (Fig. 3), and the two cyclopentane rings adopt a flattened distorted envelope and a half-chair conformation with puckering constants Δ = 19·2, 4·1°, φ_m = 26·1, −46·0°, respectively (Table 3). (Ideal values for C_s and C_2 forms are Δ = 36, 0° with φ_m = 46·7°.) The methoxycarbonyl group is in a similar orientation with respect to the C(3)—C(7) bond to the —CO₂Me group in molecule 2 of isomer (1) and is rotated by *ca* 10° with respect to the —CO₂Me group in molecule 1 of isomer (1). With the changes in configuration at C(4) and C(6) and in the conformations of both rings there are some small changes in bond angles between the isomers. The most noticeable of these are at C(7), where deviations in angles of up to 5·9° are observed. Another notable change is in angle O(2)—C(4)—C(5) (Δθ_{av} = 4·7°). Other changes

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* The crystallographic numbering system used to identify atoms is used throughout the following discussion. The chemical system is given in (1).

Table 4. *Selected bond distances (Å) and bond angles (°) with e.s.d.'s in parentheses*

| | Isomer (1) | | |
	Molecule 1	Molecule 2	Isomer (2)
O(1)–C(1)	1·22	1·22	1·203 (4)
O(2)–C(4)	1·46	1·45	1·431 (4)
O(3)–C(9)	1·35	1·34	1·321 (6)
O(3)–C(10)	1·45	1·44	1·439 (6)
O(4)–C(9)	1·22	1·20	1·182 (5)
C(1)–C(2)	1·51	1·53	1·527 (5)
C(1)–C(8)	1·51	1·49	1·507 (6)
C(2)–C(3)	1·53	1·55	1·534 (5)
C(2)–C(11)	1·56	1·54	1·542 (6)
C(2)–C(12)	1·54	1·52	1·513 (5)
C(3)–C(4)	1·52	1·52	1·520 (5)
C(3)–C(7)	1·56	1·53	1·569 (5)
C(4)–C(5)	1·50	1·52	1·507 (5)
C(5)–C(6)	1·55	1·55	1·521 (5)
C(6)–C(7)	1·57	1·59	1·563 (6)
C(6)–C(13)	1·54	1·54	1·534 (5)
C(7)–C(8)	1·56	1·55	1·531 (5)
C(7)–C(9)	1·49	1·51	1·517 (6)

$\sigma = 0.011-0.014$ Å

O(1)–C(1)–C(2)	125·2	124·9	125·5 (4)
O(1)–C(1)–C(8)	123·7	123·3	124·3 (4)
C(2)–C(1)–C(8)	111·1	111·8	110·2 (3)
C(1)–C(2)–C(3)	102·5	101·0	103·3 (3)
C(1)–C(2)–C(11)	105·7	105·5	106·1 (3)
C(1)–C(2)–C(12)	113·4	113·6	112·0 (4)
C(3)–C(2)–C(11)	109·7	109·5	110·1 (3)
C(3)–C(2)–C(12)	115·9	116·6	115·5 (3)
C(11)–C(2)–C(12)	109·0	109·9	109·3 (4)
C(2)–C(3)–C(4)	117·1	117·6	118·0 (3)
C(2)–C(3)–C(7)	107·3	108·0	107·0 (3)
C(4)–C(3)–C(7)	103·5	103·7	104·3 (3)
C(3)–C(4)–O(2)	110·1	108·6	111·5 (3)
C(3)–C(4)–C(5)	102·9	103·8	103·7 (3)
O(2)–C(4)–C(5)	107·7	108·4	112·7 (3)
C(4)–C(5)–C(6)	106·4	104·8	102·2 (3)
C(5)–C(6)–C(7)	104·4	104·3	104·8 (3)
C(5)–C(6)–C(13)	111·0	111·8	114·2 (3)
C(7)–C(6)–C(13)	116·0	114·4	116·6 (4)
C(6)–C(7)–C(3)	104·8	105·8	104·5 (3)
C(6)–C(7)–C(8)	117·7	117·5	112·4 (3)
C(6)–C(7)–C(9)	108·1	105·3	111·2 (3)
C(3)–C(7)–C(8)	102·5	104·2	106·1 (3)
C(3)–C(7)–C(9)	115·0	114·1	112·7 (3)
C(8)–C(7)–C(9)	109·0	110·2	109·7 (4)
C(7)–C(8)–C(1)	106·4	106·4	106·7 (3)
C(7)–C(9)–O(3)	112·6	112·3	112·4 (4)
C(7)–C(9)–O(4)	126·2	126·9	124·6 (5)
O(3)–C(9)–C(4)	120·9	120·8	122·9 (5)
C(9)–O(3)–C(10)	116·1	118·4	116·0 (5)

$\sigma = 0.6-1.0°$

Table 5. *Geometry of the hydrogen bonding in isomer (2) (distances in Å, angles in °)*

O(2)–H(O2)	0·99 (4)	C(4)–O(2)–H(O2)	113 (2)
O(2)···H(O2')(1−y, −z, 1−x)	1·71 (4)	···H(O2')	127 (1)
O(2)···O(2^i)(1−y, −z, 1−x)	2·687 (3)	O(2^i)···O(2)···O(2^{ii})	119·9
···O(2^{ii})(1−z, 1−x, −y)	2·687 (3)	H(O2)–O(2)···H(O2^i)	115 (4)
		O(2)–H(O2)···O(2^{ii})	172 (4)

are <3° and are not significant within the measured e.s.d.'s. The fold angle θ (Table 3) between the cyclopentane rings in both isomers is essentially the same (122–125°).

No intramolecular contacts involving the hydroxyl and the C(1)–O(1) carbonyl group are observed in isomer (2). Instead, the hydroxyl is involved in hydrogen bonding with the OH group of other molecules (Table 5) resulting in hexameric units about centers of symmetry (Fig. 4).
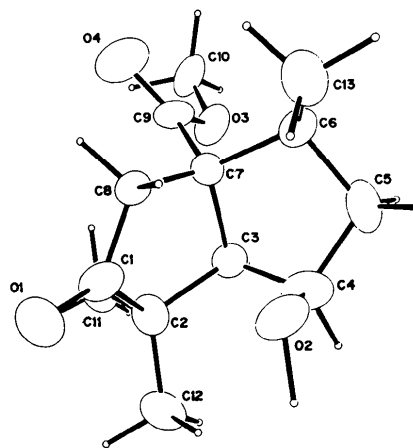

Fig. 1. *ORTEP* view (Johnson, 1965) of molecule 2 of isomer (1). Thermal ellipsoids are drawn at the 50% probability level. H atoms are drawn with uniform isotropic thermal parameters.
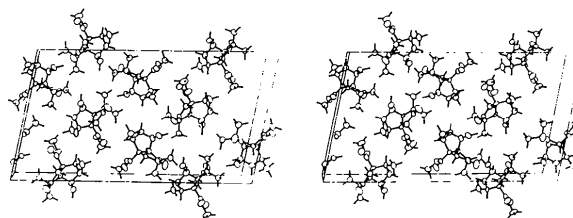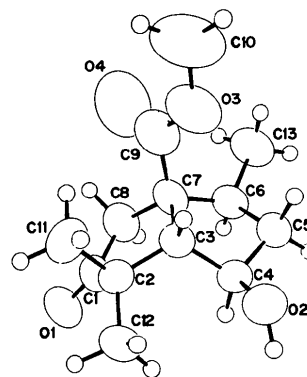

Fig. 2. Stereoscopic view down **b** of the crystal packing in isomer (1).
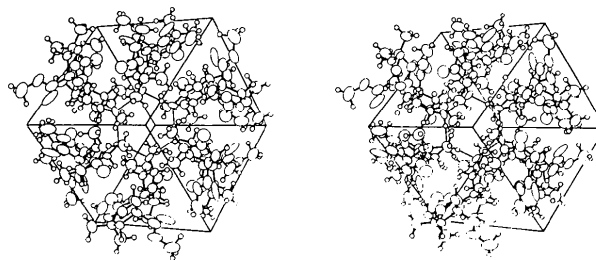

Fig. 3. *ORTEP* (Johnson, 1965) view of isomer (2).

Fig. 4. Stereoscopic view down [111] of the crystal packing in isomer (2).

It is of interest that the hydroxyl group of (5), which is the precursor of isomer (2) and is formed as the only product from the sodium borohydride reduction of (4), must have the *exo* configuration. Usually such reactions of bicyclo[3.3.0]octan-2-ones proceed with preferential attack on the *exo* face of the ketone to give the *endo* alcohol (Tabushi, Fujita & Oda, 1970; Paquette, 1979). The exclusive formation of the *endo* product in the case of (4) may result from two factors: (i) reduced steric hindrance to *endo* attack because of an increased fold angle between the rings resulting from the presence of the ethylenic bond and (ii) increased

(5)   (6)

$(E = CO_2Me)$
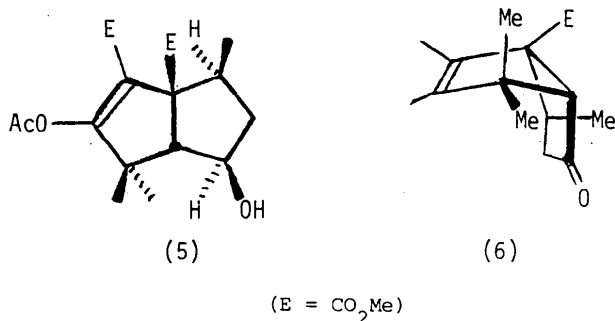
hindrance to *exo* attack because of the secondary *exo*-methyl group. These factors apply only if this methyl group has a pseudoaxial disposition and the *endo* geminal methyl group a pseudoequatorial disposition [*cf.* (6)]. It may be noted, however, that in isomer (2) both the hydroxyl and the secondary methyl

groups are pseudoequatorial with dihedral angles C(12)—C(2)···C(4)—O(2) and C(9)—C(7)···C(6)—C(13) of —46 and —21°, respectively.

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Structure of N-(2-Acetyl-3-benzofuranyl)-p-toluenesulfonamide

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Abstract. $C_{17}H_{15}NO_4S$, $M_r = 329.4$, monoclinic, $P2_1/n$, $a = 11.574$ (5), $b = 8.375$ (4), $c = 17.342$ (8) Å, $\beta = 108.0$ (3)°, $V = 1598$ (1) Å^3, $Z = 4$, $D_x = 1.369$ g cm^{-3}, $\lambda(Mo\ K\alpha) = 0.71073$ Å, $\mu = 2.11$ cm^{-1}, $F(000) = 688$, room temperature, $R = 0.045$ for 2777 observed counter reflections. The structure consists of two planar moieties, the benzofuran system and the S-aryl one, which form an angle of about 79°. There is