bond are 53·1 (7) and 52·6 (7)°, respectively, whereas those of rings *B* and *C* are 55·7 (8) and −2·2 (8)°.

Thus, *O*-methylbaccharocephol is a new member of a rare group of sesquiterpene γ-lactols with an amorphane-type of carbon skeleton (Fischer, Olivier & Fischer, 1979). The true natural product corresponds to baccharocephol (an OH group instead of OCH_3); the isolation procedure and spectroscopic data of baccharocephol, of its *O*-methyl derivative and of other diterpenoids also isolated from *B. sphaerocephala* will be published elsewhere.

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Structure of *cis*-4-Acetyl-6,6-dimethyl-3-oxabicyclo[3.1.0]hexan-2-one*

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Abstract. $C_9H_{12}O_3$, $M_r = 168·2$, orthorhombic, $P2_12_12_1$, $a = 6·814$ (1), $b = 10·632$ (1), $c = 12·183$ (1) Å, $V = 882·6$ (2) Å^3, $Z = 4$, $D_m = 1·28$, $D_x = 1·27$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0·102$ mm^{-1}, $F(000) = 360$, $T = 293$ K, $R = 0·033$ for 657 reflections. The bicyclohexane moiety adopts a boat conformation with the five-membered lactone ring having an envelope conformation. The cyclopropane ring is inclined to the five-membered ring at an angle of 69·7 (2)°. The phase angle of pseudorotation for the five-membered ring is 38·4° and the degree of puckering is 7·5°.

Introduction. (1*R*)-*cis*-Deltamethrin molecules are used as agricultural insecticides because of their high potency, low mammalian toxicity and biodegradability (Mandal, Borude, Armugasamy, Soni, Jawalkar, Mahajan, Ratnam & Goghare, 1986). In an attempt to synthesize acid moieties of deltamethrins, the title compound was prepared and is characterized by X-ray structure analysis.

Experimental. Crystals of approximate dimensions 0·62 × 0·35 × 0·25 mm; density by flotation in KI solution; lattice parameters from 24 reflections ($23 < 2\theta < 41°$); intensity data collected on Enraf–Nonius CAD-4F-11M single-crystal X-ray diffractometer, graphite-monochromated Mo $K\alpha$ radiation, $\omega/2\theta$ scan mode, scan speed 1° min^{-1}; $\theta < 23·5°$; of 851 reflections collected ($h = 0$ to 7, $k = 0$ to 11 and $l = 0$ to 13), 657 were judged significant ($|F_o| \geq 3\sigma|F_o|$). Four standard reflections (440, 314, 106 and $\bar{1}5\bar{2}$) measured every 3600 s, 3% variation in intensity; no correction for absorption; structure solved by direct methods, *MULTAN*78 (Main, Hull, Lessinger, Germain, Dec-

Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic thermal parameters for non*-H *atoms with e.s.d.'s in parentheses*

$B_{eq} = \frac{1}{3}(B_{11} + B_{22} + B_{33})$.

	x	*y*	*z*	B_{eq}(Å^2)
O(1)	2487 (3)	1614 (2)	1776 (17)	5·53
O(2)	1272 (3)	2122 (2)	5540 (2)	5·33
C(1)	1406 (4)	−273 (2)	2718 (2)	3·59
C(2)	1694 (4)	1092 (3)	2530 (2)	4·01
O(3)	876 (3)	1771 (1)	3361 (1)	4·17
C(4)	−256 (3)	974 (2)	4081 (2)	3·35
C(5)	249 (3)	−373 (2)	3776 (2)	3·21
C(6)	2353 (4)	−780 (2)	3770 (2)	3·17
C(7)	90 (4)	1328 (2)	5277 (2)	3·70
C(8)	−1138 (4)	645 (2)	6088 (2)	4·78
C(9)	2655 (5)	−2199 (2)	3778 (2)	4·56
C(10)	3991 (4)	−83 (3)	4325 (2)	4·14

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Table 2. *Bond distances* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

O(1)–C(2)	1·202 (16)	C(4)–C(5)	1·519 (3)
O(2)–C(7)	1·210 (3)	C(4)–C(7)	1·523 (4)
C(1)–C(2)	1·482 (4)	C(5)–C(6)	1·498 (4)
C(1)–C(5)	1·515 (3)	C(6)–C(9)	1·522 (3)
C(1)–C(6)	1·533 (3)	C(6)–C(10)	1·501 (4)
C(2)–O(3)	1·362 (3)	C(7)–C(8)	1·485 (4)
O(3)–C(4)	1·443 (3)		
C(2)–C(1)–C(5)	105·6 (2)	C(1)–C(5)–C(6)	61·2 (2)
C(2)–C(1)–C(6)	114·7 (2)	C(4)–C(5)–C(6)	119·4 (2)
C(5)–C(1)–C(6)	58·9 (2)	C(1)–C(6)–C(5)	60·0 (2)
O(1)–C(2)–C(1)	129·0 (6)	C(1)–C(6)–C(9)	114·2 (2)
O(1)–C(2)–O(3)	120·5 (6)	C(1)–C(6)–C(10)	121·1 (2)
C(1)–C(2)–O(3)	110·5 (2)	C(5)–C(6)–C(9)	114·6 (2)
C(2)–O(3)–C(4)	111·1 (2)	C(5)–C(6)–C(10)	124·5 (2)
O(3)–C(4)–C(5)	106·5 (2)	C(9)–C(6)–C(10)	112·7 (2)
O(3)–C(4)–C(7)	110·7 (2)	O(2)–C(7)–C(4)	121·9 (2)
C(5)–C(4)–C(7)	115·6 (2)	O(2)–C(7)–C(8)	122·7 (2)
C(1)–C(5)–C(4)	105·1 (2)	C(4)–C(7)–C(8)	115·4 (2)

lercq & Woolfson, 1978); full-matrix refinement (on F) of scale factor, positional and anisotropic thermal parameters (isotropic thermal parameters for H atoms) converged to an R of 0·033 and $wR = 0·032$, $S = 0·741$; $\sum w(|F_o| - |F_c|)^2$ minimized where $w = [4·0 + 1·0|F_o| + 0·04|F_o|^2]^{-1}$; $(\Delta/\sigma)_{max} = 0·1$; final $\Delta\rho$ excursion $\leq |0·3|$ e Å^{-3}; no correction for secondary extinction; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); *LALS* (Gantzel, Sparks & Trueblood, 1961) was used for refinement.

Discussion. The atomic parameters with their e.s.d.'s and equivalent isotropic thermal parameters are given in Table 1.* Bond lengths and bond angles involving the non-H atoms are given in Table 2. Fig. 1 gives a perspective view of the molecule along with the crystallographic numbering of atoms. The bicyclo-[3.1.0]hexane moiety adopts a boat conformation while the five-membered ring adopts an envelope conformation. As a result a global boat form ensues with the fused cyclopropane. The cyclopropane ring is inclined to the five-membered ring at an angle of 69·7 (2)°. A similar situation has been observed in *N-exo*-6-bicyclo[3.1.0]hexyl-*p*-bromobenzenesulfonamide (Grostic, Duchamp & Chidester, 1971), *N'*-isopropylidenebicyclo[3.1.0]hexane-6-*exo*-carbohydrazide (Morris, Rust & Rust, 1977) and 3,3-dichloro-7-(2,2-dichlorovinyl)tricyclo[4.1.0.0^{2,4}]heptane (Bernardinelli, Gerdil & Zuber, 1983). From a systematic analysis of the bonding characteristics of cyclopropane, it has been shown that the geometry is dependent on the type and nature of the substituents (Allen, 1981).

*Lists of structure factors, anisotropic thermal parameters, H-atom parameters and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44372 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

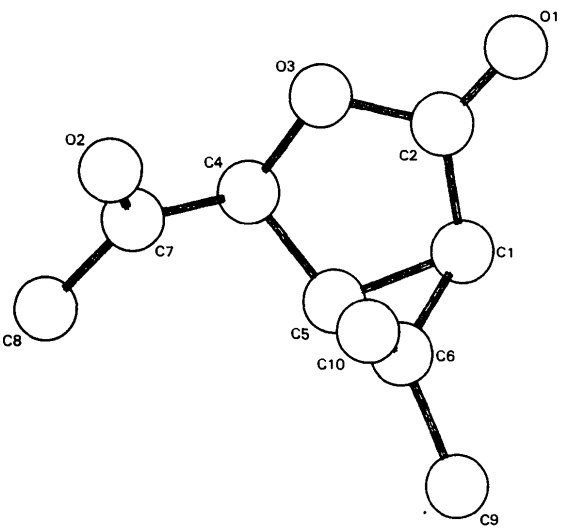

Fig. 1. A perspective view of the molecule along with the crystallographic numbering of atoms.

The average bond length of C–C = 1·515 (3) Å as found in the present study agrees with the value of 1·515 (3) Å for C(sp^3)–C(sp^3) with another C(sp^3) as substituent on the ring. The phase angle of pseudo-rotation for the five-membered lactone ring is 38·4° and the degree of puckering is 7·5° (Altona & Sundaralingam, 1972). The molecules are held together by van der Waals interactions.

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