The conformation of the aliphatic chain is *trans–trans–gauche* so the presence of one methyl group at the chain does not cause conformational variations with respect to the 1,4-butanediyl dibenzoate (Bocelli & Grenier-Loustalot, 1982*a*). It is noticeably important that the conformation of the analogous derivative with two methyls was *gauche–trans–gauche* (Bocelli & Grenier-Loustalot, 1982*b*).

Intermolecular contacts are in the range of van der Waals interactions.

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Structure and Absolute Configuration of Euphoscopin A *p*-Bromobenzoate, $C_{38}H_{43}BrO_9$, and Euphornin Acetal *p*-Bromobenzoate, $C_{37}H_{45}BrO_7$

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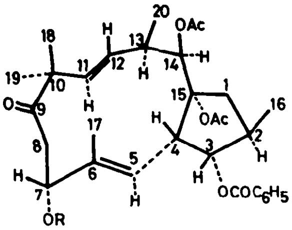
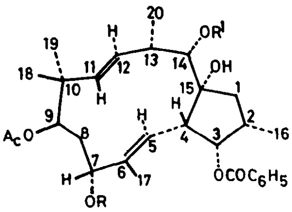
Abstract. $C_{38}H_{43}BrO_9$ (I): $M_r = 723{\cdot}7$, orthorhombic, $P2_12_12_1$, $a = 16{\cdot}271\,(2)$, $b = 23{\cdot}577\,(3)$, $c = 9{\cdot}786\,(1)$ Å, $V = 3754{\cdot}1\,(6)$ Å^3, $Z = 4$, $D_m = 1{\cdot}28\,(2)$, $D_x = 1{\cdot}28$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å, $\mu = 2{\cdot}07$ mm^{-1}, $F(000) = 1512$, $T = 298\,(1)$ K, $R = 0{\cdot}046$ for 2948 unique reflections. $C_{37}H_{45}BrO_7$ (II): $M_r = 681{\cdot}7$, monoclinic, $P2_1$, $a = 17{\cdot}104\,(3)$, $b = 13{\cdot}837\,(2)$, $c = 7{\cdot}611\,(1)$ Å, $\beta = 99{\cdot}14\,(2)°$, $V = 1778{\cdot}4\,(5)$ Å^3, $Z = 2$, $D_m = 1{\cdot}22\,(2)$, $D_x = 1{\cdot}27$ Mg m^{-3}, Mo $K\alpha_1$, $\lambda = 0{\cdot}70926$ Å, $\mu = 1{\cdot}19$ mm^{-1}, $F(000) = 716$, $T = 300\,(1)$ K, $R = 0{\cdot}036$ for 1793 unique reflections. It is confirmed that the polyoxygenated novel diterpenes euphoscopin A and euphornin have the jatrophone skeleton with the *trans* ring junction. In the two molecules three of the seven asymmetric carbon atoms have opposite absolute configurations. The molecules are held together by van der Waals forces.

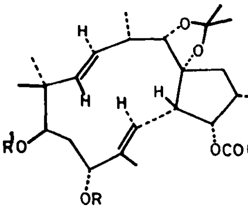
Introduction. Euphoscopins are new toxic substances isolated from the plant *Euphorbia helioscopia* L. (Yamamura, Kosemura, Ohba, Ito & Saito, 1981). Euphornin was isolated from the plant *Euphorbia maddeni* B. by Sahai, Rastogi, Jakupovic & Bohlmann (1981) and from the plant *Euphorbia helioscopia* L. (Shizuri, Kosemura, Ohtsuka, Terada, Yamamura, Ohba, Ito & Saito, 1984). The cytotoxicity of euphoscopin A is stronger than that of euphornin. Their NMR and mass spectra suggest that they have the same jatrophone skeleton with different absolute configurations. Crystals of the title compounds were subjected to X-ray crystal structure analyses to determine their absolute structures.



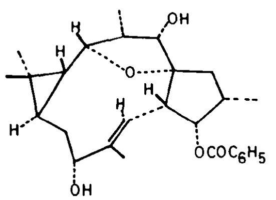
(I) R=p-BrC$_6$H$_4$CO (III) R=H



(IV) R=R^1=Ac (V) R=COCH$_2$Br, R^1=Ac
(VI) R=Ac, R^1=COCH$_2$Br



(II) R=p-BrC$_6$H$_4$CO, R^1=H
(VII) R=R^1=Ac



(VIII)

Experimental. The *p*-bromobenzoate (I) was prepared from euphoscopin A (III) in order to establish its absolute structure. Euphornin (IV), $C_{33}H_{44}O_9$, is orthorhombic, $P2_12_12_1$, $a = 18{\cdot}637$ (4), $b = 42{\cdot}053$ (8), $c = 12{\cdot}934$ (4) Å, $V = 10137$ (4) Å^3, $Z = 12$. Not enough reflections were collected to solve the structure. The bromides, (V) and (VI), showed analogous crystal data: (V) $C_{33}H_{43}BrO_9$, orthorhombic, $P2_12_12_1$, $a = 19{\cdot}4$, $b = 42{\cdot}8$, $c = 12{\cdot}5$ Å, $V = 10379$ Å^3, $Z = 12$, $D_m = D_x = 1{\cdot}27$ Mg m^{-3}; (VI) $C_{33}H_{43}BrO_9$, orthorhombic, $P2_12_12_1$, $a = 18{\cdot}590$ (4), $b = 41{\cdot}905$ (8), $c = 13{\cdot}538$ (4) Å, $V = 10546$ (4) Å^3, $Z = 12$. Crystals of (VI) decayed severely after X-ray irradiation and the higher-order reflections were too weak to be measured. A *p*-bromobenzoate was prepared from (IV) and the acetate group on C(14) and hydroxyl group on C(15) were altered into an acetal to fix the twelve-membered-ring conformation, in the hope of obtaining suitable crystals for structure analysis (Shizuri *et al.*, 1984). The crystal structure analysis of (I) and (II) was carried out to determine the absolute structures of (III) and (IV). Experimental conditions are listed in Table 1. D_m measured by flotation in aqueous solution of potassium iodide; Laue group and preliminary lattice constants determined with Weissenberg camera; Rigaku AFC-5 four-circle diffractometer, θ–2θ scan, speed 6° min^{-1} in θ; space group determined uniquely from systematic absences. Corrections for Lorentz, polarization and absorption; structures solved by Patterson–Fourier method and refined by block-diagonal least squares, anisotropic thermal parameters for non-H atoms and positional and isotropic thermal parameters of H atoms refined, $\sum w||F_o| - |F_c||^2$ minimized; complex neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974); Universal Crystallographic Computation Program System *UNICS*III (Sakurai & Kobayashi, 1979).*

Table 1. *Experimental conditions and refinement details*

	(I)	(II)
Habit of crystals	Prismatic *c*	Prismatic *c*
Solvent used for recrystallization	Ethyl acetate–acetone	Ethyl acetate–*n*-hexane
Size of specimen (mm)	0·3 × 0·3 × 0·5	0·3 × 0·3 × 0·5
Number of reflections and 2θ range (°) for measuring lattice parameters	25 $44 < 2\theta < 49$	20 $30 < 2\theta < 36$
$2\theta_{\max}$ (°)	135	50
Range of *h*, *k* and *l*	$0 \le h \le 18$ $0 \le k \le 27$ $0 \le l \le 11$	$-20 \le h \le 20$ $0 \le k \le 16$ $0 \le l \le 9$
Systematic absences	*h*00, *h* odd 0*k*0, *k* odd 00*l*, *l* odd	0*k*0, *k* odd
Variation of $\lvert F_o\rvert$ of *n* standard reflections, $\sum(\lvert F_o\rvert/\lvert F_o\rvert_{\text{initial}})/n$	$n = 4$ 0·95–1·00	$n = 5$ 0·99–1·01
Number of reflections measured	3685	3602
Number of unique reflections observed $[\lvert F_o\rvert > 3\sigma(\lvert F_o\rvert)]$	2948	1793
Number of parameters	605	586
Absorption correction, $(A^*)^{1/2}$	1·25–1·34	1·15–1·21
Number of H atoms found on difference synthesis	41	42
R	0·046	0·036
wR	0·068	0·033
$w^{-1} = \sigma^2(\lvert F_o\rvert) + (c\lvert F_o\rvert)^2$	$c = 0{\cdot}020$	$c = 0{\cdot}015$
S	2·7	1·4
$(\Delta\rho)_{\min}$ and $(\Delta\rho)_{\max}$ in final difference synthesis (e Å^{-3})	−0·73, 0·38	−0·24, 0·18
$(\Delta/\sigma)_{\max}$	0·5 for non-H, 1·0 for H	0·4 for non-H, 1·2 for H

The enantiomorphic structures of (I) and (II) gave $R = 0{\cdot}055$, $wR = 0{\cdot}080$ and $R = 0{\cdot}044$, $wR = 0{\cdot}043$, respectively. The absolute structures listed in Table 2 are correct at 0·995 significance level (Hamilton, 1965).

Discussion. Perspective drawings of (I) and (II) are shown in Fig. 1. Selected bond lengths and bond angles are listed in Table 3. The molecules consist of five-membered and twelve-membered rings. The configuration at the ring junction, C(4)—C(15), is *trans* in both (I) and (II). The double bonds in the twelve-membered ring adopt a *trans* conformation. There are seven asymmetric carbon atoms in (I). Three of them, C(2), C(13) and C(14), have different absolute configurations from the corresponding ones in (II). The torsion angle C(9)—C(10)—C(11)—C(12) of (I) and (II) is −47·3 (7) and 132·4 (5)°, respectively, the difference being 179·7 (7)°. Presumably, this is mainly due to the difference of the absolute configuration at C(13). As judged from the CD spectra of (IV) and (VII) listed in Table 4, the acetal ring formation does not change the

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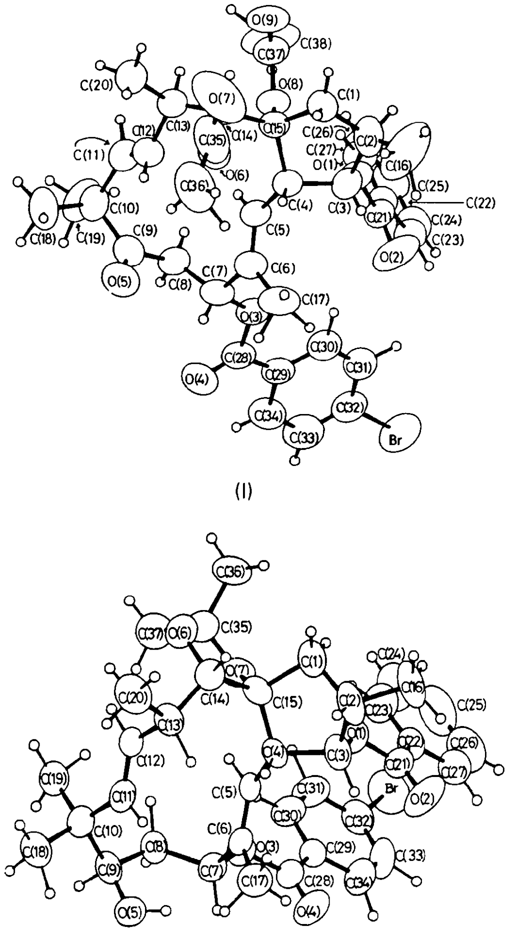
* Lists of structure factors, anisotropic thermal parameters, atomic parameters for H atoms, bond lengths involving H atoms and torsion angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39881 (61 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Positional parameters* ($\times 10^4$; *for* Br $\times 10^5$) *and equivalent isotropic thermal parameters* (*Hamilton,* 1959)

	x	y	z	B_{eq}(Å^2)
Compound (I)				
Br	54853 (4)	48188 (3)	12122 (9)	8·0
O(1)	30 (2)	4337 (1)	−388 (4)	5·3
O(2)	864 (2)	4917 (2)	748 (5)	8·2
O(3)	1866 (2)	3478 (1)	2514 (4)	5·1
O(4)	2623 (2)	3064 (2)	4159 (4)	6·8
O(5)	295 (2)	2272 (2)	4214 (4)	6·5
O(6)	−2119 (2)	3182 (1)	2285 (4)	5·1
O(7)	−3495 (2)	3270 (3)	2062 (7)	12·1
O(8)	−977 (2)	3362 (1)	−896 (3)	4·9
O(9)	−2087 (2)	3172 (2)	−2186 (4)	7·6
C(1)	−1971 (3)	4084 (2)	−85 (6)	5·5
C(2)	−1395 (3)	4586 (2)	−130 (9)	7·4
C(3)	−614 (3)	4402 (2)	608 (6)	5·0
C(4)	−807 (2)	3817 (2)	1257 (5)	4·2
C(5)	−69 (3)	3468 (2)	1599 (5)	4·2
C(6)	402 (3)	3545 (2)	2689 (5)	4·6
C(7)	1139 (3)	3168 (2)	2977 (5)	4·8
C(8)	1130 (3)	2587 (2)	2362 (5)	4·6
C(9)	518 (3)	2192 (2)	3041 (6)	4·9
C(10)	194 (3)	1686 (2)	2208 (6)	5·3
C(11)	−444 (3)	1925 (2)	1225 (6)	5·1
C(12)	−1032 (3)	2277 (2)	1595 (5)	4·9
C(13)	−1729 (3)	2458 (2)	685 (5)	5·0
C(14)	−2002 (3)	3071 (2)	836 (5)	4·6
C(15)	−1459 (2)	3560 (2)	285 (5)	4·3
C(16)	−1767 (5)	5107 (3)	442 (19)	16·8
C(17)	291 (4)	4016 (3)	3704 (7)	7·0
C(18)	−195 (4)	1249 (2)	3169 (8)	7·7
C(19)	905 (3)	1403 (2)	1450 (9)	7·6
C(20)	−2460 (3)	2058 (3)	969 (8)	6·9
C(21)	739 (3)	4601 (2)	−191 (6)	4·8
C(22)	1353 (2)	4462 (2)	−1278 (5)	4·5
C(23)	2105 (3)	4742 (2)	−1256 (6)	5·5
C(24)	2698 (3)	4619 (3)	−2234 (7)	6·3
C(25)	2535 (3)	4226 (3)	−3228 (6)	6·3
C(26)	1785 (4)	3943 (3)	−3245 (6)	6·5
C(27)	1196 (3)	4062 (2)	−2279 (6)	5·6
C(28)	2574 (3)	3378 (2)	3199 (6)	5·0
C(29)	3272 (3)	3719 (2)	2633 (6)	4·9
C(30)	3174 (3)	4108 (2)	1605 (7)	6·0
C(31)	3836 (3)	4430 (2)	1178 (7)	6·3
C(32)	4587 (3)	4353 (2)	1759 (6)	5·8
C(33)	4705 (3)	3957 (3)	2756 (8)	7·2
C(34)	4036 (3)	3637 (3)	3189 (7)	6·3
C(35)	−2896 (4)	3254 (3)	2754 (8)	7·7
C(36)	−2886 (5)	3283 (4)	4294 (8)	9·3
C(37)	−1356 (3)	3192 (3)	−2048 (6)	6·1
C(38)	−734 (5)	3016 (5)	−3069 (8)	10·9
Compound (II)				
Br	35741 (5)	0*	122627 (10)	8·1
O(1)	1544 (2)	3358 (2)	4513 (4)	4·1
O(2)	1955 (3)	2183 (4)	2883 (5)	7·9
O(3)	3916 (2)	4061 (3)	7523 (4)	4·3
O(4)	4236 (2)	3014 (3)	5504 (5)	6·0
O(5)	4659 (2)	6574 (3)	5438 (5)	6·0
O(6)	692 (2)	6814 (3)	6075 (5)	4·9
O(7)	1242 (2)	5338 (3)	6606 (4)	4·3
C(1)	415 (3)	4819 (4)	3840 (8)	5·3
C(2)	704 (4)	4299 (4)	2316 (7)	5·6
C(3)	1550 (3)	4065 (4)	3082 (7)	4·3
C(4)	1847 (3)	5016 (4)	3965 (6)	3·4
C(5)	2603 (3)	4920 (4)	5260 (6)	3·4
C(6)	3330 (3)	4944 (4)	4875 (6)	3·6
C(7)	4018 (3)	4894 (4)	6380 (7)	4·0
C(8)	4077 (3)	5734 (4)	7688 (7)	4·5
C(9)	4357 (3)	6715 (4)	7050 (8)	4·9
C(10)	3741 (3)	7535 (4)	6911 (7)	4·6
C(11)	3037 (3)	7304 (4)	5484 (7)	4·2
C(12)	2280 (3)	7368 (4)	5619 (7)	3·6
C(13)	1625 (3)	7221 (4)	4103 (7)	4·0
C(14)	968 (3)	6539 (4)	4455 (6)	3·9
C(15)	1130 (3)	5439 (4)	4732 (7)	3·8
C(16)	175 (4)	3441 (5)	1569 (8)	6·9
C(17)	3537 (3)	5036 (6)	3034 (7)	6·0
C(18)	4133 (4)	8454 (4)	6320 (9)	6·3
C(19)	3499 (3)	7714 (4)	8744 (8)	5·4
C(20)	1248 (4)	8215 (5)	3556 (8)	5·9
C(21)	1765 (3)	2446 (4)	4251 (7)	4·6
C(22)	1737 (3)	1819 (4)	5804 (7)	4·2
C(23)	1487 (4)	2161 (5)	7324 (8)	6·0
C(24)	1471 (4)	1518 (6)	8730 (9)	8·0
C(25)	1699 (4)	579 (5)	8648 (10)	8·0
C(26)	1936 (4)	258 (5)	7181 (9)	7·8
C(27)	1959 (3)	862 (5)	5705 (9)	6·0
C(28)	4038 (3)	3169 (4)	6928 (7)	4·2
C(29)	3916 (3)	2425 (4)	8233 (7)	3·9
C(30)	3642 (3)	2632 (4)	9802 (8)	5·3
C(31)	3519 (4)	1918 (5)	10991 (8)	5·9
C(32)	3718 (3)	994 (4)	10598 (7)	4·8
C(33)	3996 (4)	763 (4)	9110 (8)	5·6
C(34)	4099 (4)	1475 (4)	7907 (8)	5·4
C(35)	792 (3)	6038 (4)	7331 (7)	4·5
C(36)	−28 (3)	5673 (5)	7590 (8)	5·7
C(37)	1259 (4)	6412 (5)	9069 (7)	6·2

* This parameter was used to define the origin of the unit cell along y and is listed without e.s.d.



(I)

(II)

Fig. 1. *ORTEP* drawings (Johnson, 1965) of the molecules with thermal ellipsoids scaled at the 50% probability level. H atoms are represented by circles of radius 0·08 Å.

conformation of the original diterpene (IV). A tricyclic compound (VIII) is afforded in high yield in the hydrolysis of (IV) with K_2CO_3–MeOH (room temperature, 10 h) followed by three-membered ring

Table 3. *Selected bond lengths* (Å) *and bond angles* (°)

Compound (I)			
Br–C(32)	1·905 (5)	C(6)–C(7)	1·519 (7)
O(1)–C(3)	1·439 (6)	C(6)–C(17)	1·501 (8)
O(3)–C(7)	1·462 (6)	C(7)–C(8)	1·496 (7)
O(5)–C(9)	1·219 (7)	C(8)–C(9)	1·517 (7)
O(6)–C(14)	1·454 (6)	C(9)–C(10)	1·538 (7)
O(8)–C(15)	1·473 (5)	C(10)–C(11)	1·523 (7)
C(1)–C(2)	1·510 (7)	C(10)–C(18)	1·532 (8)
C(1)–C(15)	1·533 (7)	C(10)–C(19)	1·528 (8)
C(2)–C(3)	1·525 (8)	C(11)–C(12)	1·317 (7)
C(2)–C(16)	1·479 (11)	C(12)–C(13)	1·504 (7)
C(3)–C(4)	1·551 (7)	C(13)–C(14)	1·519 (7)
C(4)–C(5)	1·494 (6)	C(13)–C(20)	1·543 (8)
C(4)–C(15)	1·548 (6)	C(14)–C(15)	1·549 (6)
C(5)–C(6)	1·326 (7)		
C(2)–C(1)–C(15)	107·5 (4)	C(9)–C(10)–C(11)	106·3 (4)
C(1)–C(2)–C(3)	106·3 (4)	C(9)–C(10)–C(18)	109·8 (5)
C(1)–C(2)–C(16)	112·7 (5)	C(9)–C(10)–C(19)	109·7 (4)
C(3)–C(2)–C(16)	113·5 (6)	C(11)–C(10)–C(18)	110·8 (4)
O(1)–C(3)–C(2)	108·4 (5)	C(11)–C(10)–C(19)	111·8 (5)
O(1)–C(3)–C(4)	109·3 (4)	C(18)–C(10)–C(19)	108·5 (4)
C(2)–C(3)–C(4)	106·2 (4)	C(10)–C(11)–C(12)	123·7 (5)
C(3)–C(4)–C(5)	114·8 (3)	C(11)–C(12)–C(13)	124·3 (5)
C(3)–C(4)–C(15)	103·6 (4)	C(12)–C(13)–C(14)	115·7 (4)
C(5)–C(4)–C(15)	118·2 (4)	C(12)–C(13)–C(20)	107·5 (4)
C(4)–C(5)–C(6)	124·7 (4)	C(14)–C(13)–C(20)	109·8 (4)
C(5)–C(6)–C(7)	121·7 (4)	O(6)–C(14)–C(13)	107·7 (4)
C(5)–C(6)–C(17)	124·3 (5)	O(6)–C(14)–C(15)	106·3 (4)
C(7)–C(6)–C(17)	113·9 (4)	C(13)–C(14)–C(15)	120·5 (4)
O(3)–C(7)–C(6)	106·8 (4)	O(8)–C(15)–C(1)	111·1 (4)
O(3)–C(7)–C(8)	109·9 (4)	O(8)–C(15)–C(4)	104·0 (3)
C(6)–C(7)–C(8)	117·0 (4)	O(8)–C(15)–C(14)	109·9 (4)
C(7)–C(8)–C(9)	113·1 (4)	C(1)–C(15)–C(4)	101·7 (4)
O(5)–C(9)–C(8)	120·9 (4)	C(1)–C(15)–C(14)	111·8 (3)
O(5)–C(9)–C(10)	121·1 (4)	C(4)–C(15)–C(14)	117·9 (4)
C(8)–C(9)–C(10)	118·0 (5)		
Compound (II)			
Br–C(32)	1·912 (6)	C(6)–C(7)	1·508 (7)
O(1)–C(3)	1·465 (6)	C(6)–C(17)	1·504 (7)
O(3)–C(7)	1·471 (7)	C(7)–C(8)	1·523 (8)
O(5)–C(9)	1·418 (7)	C(8)–C(9)	1·543 (8)
O(6)–C(14)	1·440 (6)	C(9)–C(10)	1·541 (8)
O(6)–C(35)	1·430 (7)	C(10)–C(11)	1·522 (7)
O(7)–C(15)	1·416 (6)	C(10)–C(18)	1·538 (8)
O(7)–C(35)	1·404 (7)	C(10)–C(19)	1·537 (8)
C(1)–C(2)	1·513 (9)	C(11)–C(12)	1·318 (7)
C(1)–C(15)	1·558 (7)	C(12)–C(13)	1·489 (7)
C(2)–C(3)	1·507 (8)	C(13)–C(14)	1·523 (8)
C(2)–C(16)	1·545 (9)	C(13)–C(20)	1·548 (9)
C(3)–C(4)	1·527 (8)	C(14)–C(15)	1·555 (8)
C(4)–C(5)	1·502 (6)	C(35)–C(36)	1·533 (8)
C(4)–C(15)	1·554 (8)	C(35)–C(37)	1·523 (7)
C(5)–C(6)	1·322 (7)		
C(14)–O(6)–C(35)	110·7 (4)	C(8)–C(9)–C(10)	115·2 (4)
C(15)–O(7)–C(35)	109·5 (4)	C(9)–C(10)–C(11)	110·4 (4)
C(2)–C(1)–C(15)	105·5 (4)	C(9)–C(10)–C(18)	107·7 (4)
C(1)–C(2)–C(3)	102·5 (4)	C(9)–C(10)–C(19)	109·6 (4)
C(1)–C(2)–C(16)	113·8 (5)	C(11)–C(10)–C(18)	107·3 (4)
C(3)–C(2)–C(16)	116·6 (5)	C(11)–C(10)–C(19)	112·6 (4)
O(1)–C(3)–C(2)	108·1 (4)	C(18)–C(10)–C(19)	109·0 (5)
O(1)–C(3)–C(4)	106·8 (4)	C(10)–C(11)–C(12)	127·3 (5)
C(2)–C(3)–C(4)	102·5 (4)	C(11)–C(12)–C(13)	123·9 (5)
C(3)–C(4)–C(5)	113·8 (4)	C(12)–C(13)–C(14)	115·7 (4)
C(3)–C(4)–C(15)	105·2 (4)	C(12)–C(13)–C(20)	108·5 (5)
C(5)–C(4)–C(15)	115·8 (4)	C(14)–C(13)–C(20)	108·1 (4)
C(4)–C(5)–C(6)	126·4 (4)	O(6)–C(14)–C(13)	109·8 (4)
C(5)–C(6)–C(7)	118·6 (4)	O(6)–C(14)–C(15)	102·6 (4)
C(5)–C(6)–C(17)	125·3 (4)	C(13)–C(14)–C(15)	120·6 (4)
C(7)–C(6)–C(17)	116·2 (4)	O(7)–C(15)–C(1)	110·8 (4)
O(3)–C(7)–C(6)	109·5 (4)	O(7)–C(15)–C(4)	110·7 (4)
O(3)–C(7)–C(8)	102·3 (4)	O(7)–C(15)–C(14)	103·1 (4)
C(6)–C(7)–C(8)	115·1 (4)	C(1)–C(15)–C(4)	103·9 (4)
C(7)–C(8)–C(9)	117·2 (5)	C(1)–C(15)–C(14)	111·7 (4)
O(5)–C(9)–C(8)	109·0 (4)	C(4)–C(15)–C(14)	116·9 (5)
O(5)–C(9)–C(10)	112·4 (4)		

Table 4. *CD spectral data measured in methanol* ($c = 30–100\ \text{g m}^{-3}$) *at* 299 K

	λ_{max}(nm)	$\Delta\varepsilon$
(I)	210	−20·6
	243*	17·5
(II)	209	−21·2
	228	15·2
	246*	−11·6
(IV)	204	−43·6
	228	8·85
(VII)	205	−18·6
	229	8·74

* This absorption may be due to two benzoates.

formation using *p*-TsOH–acetone (room temperature, 5·5 h), suggesting that the torsion angle C(9)—C(10)—C(11)—H(C11) of (IV) is almost the same as that of (II). In fact, molecular-mechanics calculations for (III) and (IV) (Shizuri, Kosemura, Ohtsuka, Terada, Yamamura, Ohba, Ito & Saito, 1985) are for the most part compatible with the conformations of (I) and (II) determined by X-ray analyses. So the differences in the spectral and chemical properties of the two diterpenes (III) and (IV) can be well understood by the difference in the conformations of the twelve-membered rings.

The crystal structure consists of discrete molecules separated by normal van der Waals distances. The shortest intermolecular distances are 3·251 (7) Å for O(2)···C(24) ($\frac{1}{2} - x,\ 1 - y,\ \frac{1}{2} + z$) and 2·914 (6) Å for O(4)···O(5) ($1 - x,\ -\frac{1}{2} + y,\ 1 - z$), which is not a hydrogen bond, for (I) and (II), respectively.

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