C(6)—C(7)—C(8)	120.3 (3)	120.5 (3)
C(7)—C(8)—C(9)	121.1 (3)	121.1 (3)
C(1)—C(9)—C(8)	122.4 (2)	122.3 (3)
C(1)—C(9)—C(10)	119.6 (2)	119.4 (3)
C(8)—C(9)—C(10)	117.9 (2)	118.3 (3)
C(4)—C(10)—C(5)	122.1 (2)	122.7 (3)
C(4)—C(10)—C(9)	118.5 (2)	118.4 (3)
C(5)—C(10)—C(9)	119.5 (2)	118.9 (3)
C(1)—C(11)—C(12)	120.1 (3)	119.9 (2)
C(1)—C(11)—C(19)	120.6 (3)	121.5 (2)
C(12)—C(11)—C(19)	119.2 (3)	118.5 (2)
O(2)—C(12)—C(11)	122.6 (3)	122.2 (3)
O(2)—C(12)—C(13)	116.3 (3)	115.7 (3)
C(11)—C(12)—C(13)	121.1 (3)	122.1 (3)
C(12)—C(13)—C(14)	120.2 (4)	120.1 (3)
C(13)—C(14)—C(20)	121.5 (4)	121.2 (3)
C(16)—C(15)—C(20)	121.2 (4)	121.2 (3)
C(15)—C(16)—C(17)	120.4 (4)	119.9 (3)
C(16)—C(17)—C(18)	120.3 (3)	120.7 (3)
C(17)—C(18)—C(19)	122.0 (3)	121.0 (3)
C(11)—C(19)—C(18)	122.4 (3)	122.2 (3)
C(11)—C(19)—C(20)	119.8 (3)	119.7 (2)
C(18)—C(19)—C(20)	117.8 (3)	118.1 (3)
C(14)—C(20)—C(15)	123.6 (3)	122.5 (2)
C(14)—C(20)—C(19)	118.2 (3)	118.4 (2)
C(15)—C(20)—C(19)	118.2 (3)	119.0 (2)
C(2)—O(1)—H(2)	111 (3)	106 (2)
C(12)—O(2)—H(12)	106 (2)	115 (2)

Data collection and cell refinement: Rigaku AFC-5 software (1977). Data reduction: *NTDATAIN* (Tanaka, 1979). Program used to solve structure: *MULTAN*11/84 (Main, Germain & Woolfson, 1984). Programs used to refine structure (block-diagonal least squares): *HBLS*-V and *DAPH* (Ashida, 1973). Software used to prepare material for publication: *MOLCON* (Fujii, 1979); *ORTEP*II (Johnson, 1971). Computations were carried out at the Research Center for Protein Engineering, Institute for Protein Research, Osaka University, and at the Okayama University Computer Center.

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, and bond distances and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55956 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: OH1012]

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Structure of 6-*O*-Methylerythromycin A (Clarithromycin)

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Abstract

The absolute configuration of the asymmetric centers in clarithromycin is the same as that in erythromycin A [Harris, McGeachin & Mills (1965). *Tetrahedron Lett.* pp. 679–685; Oliver & Strickland (1986). *Acta Cryst.* C**42**, 952–956]. The molecular structure is similar to that of erythromycin A. The carbonyl and the hydroxyl groups of the 14-membered aglycone are on the same side of the aglycone ring, and the 6-*O*-methyl group is in this hydrophilic region.

Comment

Clarithromycin, (I), a new semisynthetic macrolide antibiotic, has been clinically used for the treatment of infectious diseases caused by aerobic gram-positive bacteria, some gram-negative bacteria, anaerobic bacteria, *Mycoplasma* and *Chlamydia*. This antibiotic shows a similar antibacterial spectrum to erythromycin A, and its activity is twofold higher than that of erythromycin A *in vitro*. It exhibits much higher *in vivo* activity than erythromycin A because of its superior pharmacokinetic properties (Morimoto, Misawa, Adachi, Nagate, Watanabe & Omura, 1990; Morimoto, Nagate,

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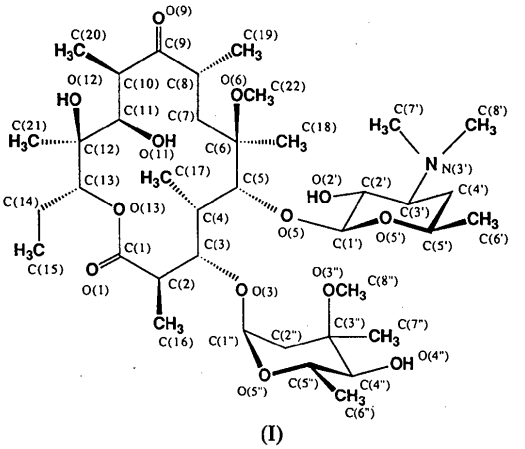
Sugita, Ono, Numata, Miyachi, Misawa, Yamada & Omura, 1990).



(I)

The absolute structure, shown in Fig. 1, was assigned on the basis of the known absolute configuration of the sugar moieties, cladinose and desosamine (Lemal, Pacht & Woodward, 1962; Richardson, 1963). The asymmetric centers of the aglycone have 2*R*, 3*S*, 4*S*, 5*R*, 6*R*, 8*R*, 10*R*, 11*R*, 12*S* and 13*R* configurations, which are the same as those established for erythromycin A.

The molecular structure is similar to that of erythromycin A and that of (14*R*)-14-hydroxy-6-*O*-methylerythromycin A (Adachi, Morimoto, Watanabe, Kamiya & Iwasaki, 1990); the structures of the 14-membered aglycone in these and the title compound can be superposed. The carbonyl groups on C(1) and C(9) and the hydroxyl group on C(11) are on the same side of the 14-membered aglycone, and the 6-*O*-methyl group is in this hydrophilic region. The carbonyl O atom O(9) makes an intramolecular hydrogen bond with O(11) [O(9)···O(11) 2.857 (4), H(O11)···O(9) 2.09 (4) Å, O(9)···H(O11)—O(11) 147 (3)°].

From the viewpoint of the structure–activity relationship, several 'diamond lattice' conformational models have been proposed for the aglycones of the 14-membered macrolide antibiotics (Nakagawa & Ōmura, 1984). The conformation of the aglycone of clarithromycin is very similar to a Perun's model III proposed for the aglycone of erythromycin B (Egan, Perun, Martin & Mitscher, 1973).

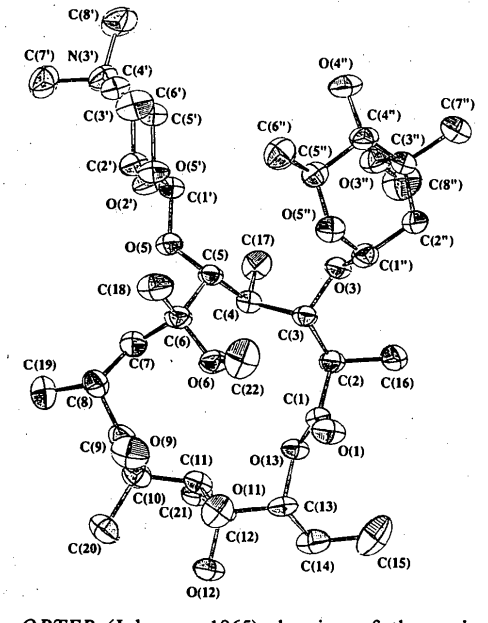


Fig. 1. *ORTEP* (Johnson, 1965) drawing of the molecule of clarithromycin. H atoms are omitted for clarity.

Experimental

Crystal data

$C_{38}H_{69}NO_{13}.CH_4O$
M_r = 780.01
Orthorhombic
$P2_12_12_1$
a = 19.979 (2) Å
b = 24.115 (3) Å
c = 8.9980 (14) Å
V = 4335 (1) Å^3
Z = 4
D_x = 1.195 Mg m^{-3}
D_m = 1.189 Mg m^{-3}
Density measured by flotation in CCl_4/*n*-hexane
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 24 reflections
θ = 15.2–17.3°
μ = 0.084 mm^{-1}
T = 296 K
Rod
0.65 × 0.5 × 0.5 mm
Colourless
Crystal source: from methanolic solution

Data collection

Rigaku AFC-4 diffractometer
ω scans
Absorption correction: none
5577 measured reflections
5577 independent reflections
4006 observed reflections [$F_o > 3\sigma(F_o)$]
R_{int} = 0
θ_{max} = 27.5°
$h = 0 \rightarrow 25$
$k = 0 \rightarrow 31$
$l = 0 \rightarrow 11$
3 standard reflections monitored every 100 reflections
intensity variation: <1%

Refinement

Refinement on F
Final R = 0.045
wR = 0.053
S = 0.7823
4006 reflections
780 parameters
All H-atom parameters refined
w = 0.5 for $|F_o| < 7.0$; 1.0 for $7.0 \leq |F_o| < 25.0$; $(25.0/|F_o|)^2$ for $25.0 \leq |F_o|$
$(\Delta/\sigma)_{max}$ = 0.35
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Tables 2.2A and 2.2C)

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

$B_{eq} = \frac{4}{3}\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
C(1)	0.0301 (2)	0.2381 (1)	0.4330 (4)	3.0 (4)
C(2)	0.0062 (2)	0.2973 (1)	0.4602 (4)	3.4 (4)
C(3)	0.0107 (2)	0.3313 (1)	0.3132 (3)	2.7 (4)
C(4)	0.0799 (2)	0.3606 (1)	0.3040 (4)	2.9 (4)
C(5)	0.1002 (2)	0.3753 (1)	0.1428 (4)	2.8 (3)
C(6)	0.1362 (2)	0.3270 (1)	0.0553 (4)	3.4 (4)
C(7)	0.2081 (2)	0.3197 (1)	0.1119 (5)	4.2 (4)
C(8)	0.2512 (2)	0.2761 (2)	0.0304 (5)	4.7 (5)
C(9)	0.2319 (2)	0.2169 (1)	0.0700 (4)	4.0 (4)
C(10)	0.2446 (2)	0.1970 (1)	0.2282 (4)	3.7 (5)
C(11)	0.1772 (2)	0.1827 (1)	0.2998 (4)	3.3 (4)
C(12)	0.1786 (2)	0.1697 (1)	0.4677 (4)	3.2 (3)
C(13)	0.1061 (2)	0.1676 (1)	0.5250 (4)	3.1 (4)
C(14)	0.0966 (2)	0.1450 (1)	0.6809 (4)	4.4 (5)
C(15)	0.0231 (3)	0.1399 (2)	0.7206 (5)	6.7 (6)
C(16)	−0.0650 (2)	0.2933 (2)	0.5218 (6)	5.8 (5)
C(17)	0.0790 (2)	0.4120 (1)	0.4041 (4)	3.9 (4)
C(18)	0.1348 (2)	0.3405 (2)	−0.1099 (4)	5.1 (6)
C(19)	0.3259 (2)	0.2863 (2)	0.0644 (8)	7.3 (6)
C(20)	0.2946 (2)	0.1483 (2)	0.2211 (5)	5.1 (5)
C(21)	0.2203 (2)	0.2111 (1)	0.5550 (4)	4.0 (4)
C(22)	0.0508 (3)	0.2565 (2)	−0.0039 (6)	6.0 (6)
O(1)	0.0054 (1)	0.2072 (1)	0.3440 (3)	4.4 (3)
O(3)	−0.0411 (1)	0.3722 (1)	0.3088 (3)	3.1 (2)
O(5)	0.1486 (1)	0.4197 (1)	0.1427 (3)	3.4 (2)
O(6)	0.1032 (1)	0.2751 (1)	0.0903 (3)	3.7 (3)
O(9)	0.2099 (2)	0.1856 (1)	−0.0226 (3)	5.7 (3)
O(11)	0.1459 (1)	0.1367 (1)	0.2292 (3)	4.5 (3)
O(12)	0.2088 (1)	0.1166 (1)	0.4939 (3)	3.9 (3)
O(13)	0.0800 (1)	0.2247 (1)	0.5250 (3)	3.1 (2)
C(1′)	0.1279 (2)	0.4714 (1)	0.0931 (4)	3.0 (4)
C(2′)	0.1802 (2)	0.5142 (1)	0.1396 (4)	3.5 (4)
C(3′)	0.1594 (2)	0.5705 (1)	0.0765 (4)	3.2 (4)
C(4′)	0.1534 (2)	0.5662 (1)	−0.0907 (4)	3.6 (4)
C(5′)	0.1037 (2)	0.5213 (1)	−0.1305 (4)	3.5 (4)
C(6′)	0.0991 (2)	0.5111 (2)	−0.2967 (4)	5.1 (5)
C(7′)	0.1705 (2)	0.6683 (1)	0.1310 (6)	5.6 (5)
C(8′)	0.2680 (2)	0.6162 (2)	0.0640 (5)	5.2 (5)
N(3′)	0.2026 (2)	0.6142 (1)	0.1368 (3)	3.9 (4)
O(2′)	0.1848 (2)	0.5160 (1)	0.2958 (3)	5.0 (3)
O(5′)	0.1236 (1)	0.4695 (1)	−0.0639 (3)	3.7 (3)
C(1″)	−0.0941 (2)	0.3627 (1)	0.2072 (4)	3.4 (4)
C(2″)	−0.1570 (2)	0.3918 (1)	0.2600 (4)	3.9 (5)
C(3″)	−0.1549 (2)	0.4553 (1)	0.2442 (4)	3.9 (5)
C(4″)	−0.1317 (2)	0.4691 (1)	0.0875 (4)	3.6 (4)
C(5″)	−0.0687 (2)	0.4377 (1)	0.0414 (4)	3.4 (4)
C(6″)	−0.0528 (2)	0.4452 (2)	−0.1219 (5)	4.8 (5)
C(7″)	−0.2236 (2)	0.4806 (2)	0.2762 (6)	6.3 (6)
C(8″)	−0.1105 (3)	0.4728 (2)	0.4917 (5)	6.7 (6)
O(3″)	−0.1043 (1)	0.4801 (1)	0.3360 (3)	4.3 (3)
O(4″)	−0.1197 (1)	0.5274 (1)	0.0700 (3)	4.4 (3)
O(5″)	−0.0765 (1)	0.3785 (1)	0.0619 (3)	3.7 (2)
C(23)(solv.)	−0.0151 (3)	0.0798 (2)	0.1337 (6)	7.3 (10)
O(23)(solv.)	0.0040 (2)	0.0848 (1)	0.2814 (4)	7.5 (5)

Table 2. *Geometric parameters* (Å, °)

C(1)—C(2)	1.526 (5)	C(14)—C(15)	1.518 (7)
C(1)—O(1)	1.200 (4)	C(22)—O(6)	1.419 (6)
C(1)—O(13)	1.335 (4)	O(3)—C(1″)	1.417 (4)
C(2)—C(3)	1.558 (5)	O(5)—C(1′)	1.387 (4)
C(2)—C(16)	1.529 (6)	C(1′)—C(2′)	1.525 (5)
C(3)—C(4)	1.554 (4)	C(1′)—O(5′)	1.415 (4)
C(3)—O(3)	1.430 (4)	C(2′)—C(3′)	1.530 (5)
C(4)—C(5)	1.548 (5)	C(2′)—O(2′)	1.409 (5)
C(4)—C(17)	1.533 (5)	C(3′)—C(4′)	1.513 (5)
C(5)—C(6)	1.579 (5)	C(3′)—N(3′)	1.467 (5)
C(5)—O(5)	1.444 (4)	C(4′)—C(5′)	1.512 (5)
C(6)—C(7)	1.534 (5)	C(5′)—C(6′)	1.519 (6)
C(6)—C(18)	1.523 (6)	C(5′)—O(5′)	1.443 (4)
C(6)—O(6)	1.448 (4)	C(7′)—N(3′)	1.454 (6)
C(7)—C(8)	1.545 (6)	C(8′)—N(3′)	1.461 (6)
C(8)—C(9)	1.521 (6)	C(1″)—C(2″)	1.517 (5)
C(8)—C(19)	1.543 (8)	C(1″)—O(5″)	1.406 (4)
C(9)—C(10)	1.523 (5)	C(2″)—C(3″)	1.538 (6)
C(9)—O(9)	1.207 (5)	C(3″)—C(4″)	1.520 (6)
C(10)—C(11)	1.531 (5)	C(3″)—C(7″)	1.529 (7)
C(10)—C(20)	1.544 (6)	C(3″)—O(3″)	1.436 (5)
C(11)—C(12)	1.543 (5)	C(4″)—C(5″)	1.527 (5)
C(11)—O(11)	1.423 (4)	C(4″)—O(4″)	1.435 (5)
C(12)—C(13)	1.539 (5)	C(5″)—C(6″)	1.515 (5)
C(12)—C(21)	1.519 (5)	C(5″)—O(5″)	1.447 (4)
C(12)—O(12)	1.435 (4)	C(8″)—O(3″)	1.417 (6)
C(13)—C(14)	1.516 (5)	C(23)—O(23)	1.388 (7)
C(13)—O(13)	1.474 (4)		

C(2)—C(1)—O(1)	124.0 (3)	C(10)—C(11)—C(12)	116.2 (3)
C(2)—C(1)—O(13)	111.1 (3)	C(10)—C(11)—O(11)	112.0 (3)
O(1)—C(1)—O(13)	124.8 (3)	C(12)—C(11)—O(11)	106.7 (3)
C(1)—C(2)—C(3)	109.8 (3)	C(11)—C(12)—C(13)	108.5 (3)
C(1)—C(2)—C(16)	106.8 (3)	C(11)—C(12)—C(21)	112.5 (3)
C(3)—C(2)—C(16)	113.2 (3)	C(11)—C(12)—O(12)	110.5 (3)
C(2)—C(3)—C(4)	109.6 (3)	C(13)—C(12)—C(21)	111.3 (3)
C(2)—C(3)—O(3)	110.1 (3)	C(13)—C(12)—O(12)	108.1 (3)
C(4)—C(3)—O(3)	109.2 (2)	C(21)—C(12)—O(12)	105.8 (3)
C(3)—C(4)—C(5)	112.8 (3)	C(12)—C(13)—C(14)	116.0 (3)
C(3)—C(4)—C(17)	109.1 (3)	C(12)—C(13)—O(13)	107.6 (3)
C(14)—C(13)—O(13)	107.0 (3)	C(3′)—C(2′)—O(2′)	111.1 (3)
C(13)—C(14)—C(15)	111.6 (4)	C(2′)—C(3′)—C(4′)	109.3 (3)
C(3)—O(3)—C(1″)	116.6 (2)	C(2′)—C(3′)—N(3′)	110.0 (3)
C(5)—O(5)—C(1′)	117.9 (3)	C(4′)—C(3′)—N(3′)	117.6 (3)
C(6)—O(6)—C(22)	118.7 (3)	C(3′)—C(4′)—C(5′)	109.7 (3)
C(1)—O(13)—C(13)	119.3 (3)	C(4′)—C(5′)—C(6′)	112.9 (3)
O(5)—C(1′)—C(2′)	108.4 (3)	C(4′)—C(5′)—O(5′)	109.9 (3)
O(5)—C(1′)—O(5′)	108.0 (3)	C(6′)—C(5′)—O(5′)	106.6 (3)
C(2′)—C(1′)—O(5′)	109.8 (3)	C(3′)—N(3′)—C(7′)	111.8 (3)
C(1′)—C(2′)—C(3′)	108.2 (3)	C(3′)—N(3′)—C(8′)	112.6 (3)
C(1′)—C(2′)—O(2′)	109.9 (3)	C(7′)—N(3′)—C(8′)	110.5 (3)
C(5)—C(4)—C(17)	111.6 (3)	C(1′)—O(5′)—C(5′)	113.7 (3)
C(4)—C(5)—C(6)	114.7 (3)	O(3)—C(1″)—C(2″)	109.9 (3)
C(4)—C(5)—O(5)	110.3 (3)	O(3)—C(1″)—O(5″)	111.7 (3)
C(6)—C(5)—O(5)	104.0 (3)	C(2″)—C(1″)—O(5″)	111.9 (3)
C(5)—C(6)—C(7)	110.3 (3)	C(1″)—C(2″)—C(3″)	114.2 (3)
C(5)—C(6)—C(18)	108.7 (3)	C(2″)—C(3″)—C(4″)	108.2 (3)
C(5)—C(6)—O(6)	108.7 (3)	C(2″)—C(3″)—C(7″)	110.9 (4)
C(7)—C(6)—C(18)	111.4 (3)	C(2″)—C(3″)—O(3″)	112.3 (3)
C(7)—C(6)—O(6)	104.8 (3)	C(4″)—C(3″)—C(7″)	111.1 (4)
C(18)—C(6)—O(6)	112.9 (3)	C(4″)—C(3″)—O(3″)	103.2 (3)
C(6)—C(7)—C(8)	116.3 (3)	C(7″)—C(3″)—O(3″)	110.9 (3)
C(7)—C(8)—C(9)	112.8 (3)	C(3″)—C(4″)—C(5″)	113.2 (3)
C(7)—C(8)—C(19)	109.7 (4)	C(3″)—C(4″)—O(4″)	111.6 (3)
C(9)—C(8)—C(19)	110.4 (4)	C(5″)—C(4″)—O(4″)	108.6 (3)
C(8)—C(9)—C(10)	118.2 (3)	C(4″)—C(5″)—C(6″)	112.1 (3)
C(8)—C(9)—O(9)	121.2 (4)	C(4″)—C(5″)—O(5″)	111.5 (3)
C(10)—C(9)—O(9)	120.6 (3)	C(6″)—C(5″)—O(5″)	105.3 (3)
C(9)—C(10)—C(11)	108.6 (3)	C(3″)—O(3″)—C(8″)	117.1 (3)
C(9)—C(10)—C(20)	107.9 (3)	C(1″)—O(5″)—C(5″)	114.4 (3)
C(11)—C(10)—C(20)	114.5 (3)		

The structure was solved by direct methods using *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), and refined by block-diagonal least-squares method. A solvate molecule and H atoms, except for H(O23), were located in a difference Fourier map. H(O23) was placed at a calculated position [O(23)—H···O(1) 180°, O—H 0.9 Å]. Calculations were performed on a FACOM M-780 computer of RIKEN using the *UNICS* III program system (Sakurai & Kobayashi, 1979).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bond distances, bond angles and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55963 (27 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: OH1013]

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Structure of a Pyrano[2,3-*b*]indolizine

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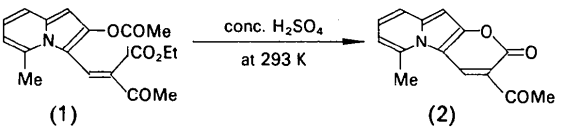
Abstract

The pyrrole and pyridine rings in the indolizine skeleton of 3-acetyl-6-methyl-2*H*-pyrano[2,3-*b*]indolizin-2-one are planar [mean deviations 0.003 (2) and 0.003 (2) Å, respectively] and inclined at 0.5 (2)° to one another. The planar [mean deviation 0.004 (2) Å] 2-pyrone ring, fused at the 2 and 3 positions of the indolizine ring, is also coplanar with the indolizine ring [dihedral angle 1.1 (2)°]. The delocalized ring system extends to the fused pyrone ring as indicated by the shortened C4—C3 bond of 1.375 (3) Å. The acetyl group at the 3 position is also coplanar with the pyrone ring [dihedral angle 0.5 (2)°].

Comment

Treatment of ethyl 2-acetyl-3-(2-acetoxy-5-methylindolizin-3-yl)acrylate (1) (329 mg, 1 mmol) with concentrated sulfuric acid (1 ml) at room temperature for 12 h gave the title compound 3-acetyl-6-methyl-2*H*-pyrano[2,3-*b*]indolizin-2-one (2) in a 12% yield (Kakehi, Ito, Murakami & Sano, 1984).



(1) (2)

The present study was undertaken to confirm the chemical structure of the title compound and to compare the structural features of many indolizine derivatives of physicochemical and pharmaceutical interest. The bond distances and angles for the indolizine skeleton in the title compound are closer to those of 1-acetoxy-2,3-diphenylindolizine (Wadsworth, Bender, Smith, Luss & Weidner, 1986) and ethyl 1-trifluoromethylindolizine-3-carboxylate (Pritchard, 1988), than to those of ethyl 3,4-dihydrocyclopenta[*hi*]indolizine-1-carboxylate (Kakehi, Kitajima, Ito & Takusagawa, 1992); this is because, in contrast to the annelation of a five-membered ring at the 1 and 8 positions of an indolizine ring, the less-hindered pyrone ring attached to the 2 and 3 positions does not cause a large distortion of the skeleton. On the other hand, the distances and angles for the 2-pyrone ring are similar to those found in various 2-pyrone derivatives (Thailambal & Vasantha Pattabhi, 1987; Thailambal, Vasantha Pattabhi & Gabe, 1986), except for the shortened C3—C4 and lengthened C4—C11 bonds. The shortening of the C3—C4 bond suggests that the 2-pyrone moiety of the title compound (2) has a different resonance structure from pyrone itself because the fused indolizine ring changes the resonance system of the pyrone moiety. Compared with the pyrone moiety in coumarin (Gavuzzo, Mazza & Giglio, 1974) and coumarin derivatives (Vasudevan, Puttaraja & Kulkarni, 1991), the pyrone ring in (2) is again characterized by its shortened C3—C4 and lengthened O1—C1 bonds, reflecting the difference between the aromatic systems of the indolizine and the benzene. The widening [129.5 (2)°] of the angle C2—C1—O2 in the pyrone moiety in (2) is probably enhanced by the steric interactions between the 3-acetyl group and O2. Such widening was observed in the case of 3-acetyl-4-hydroxy-6-phenyl-2-pyrone (Thailambal & Vasantha Pattabhi, 1985). A comparison of selected bond lengths and angles for the 2-pyrone moieties in the title compound (2) and other 2-pyrone and coumarin derivatives is summarized in Table 3.

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