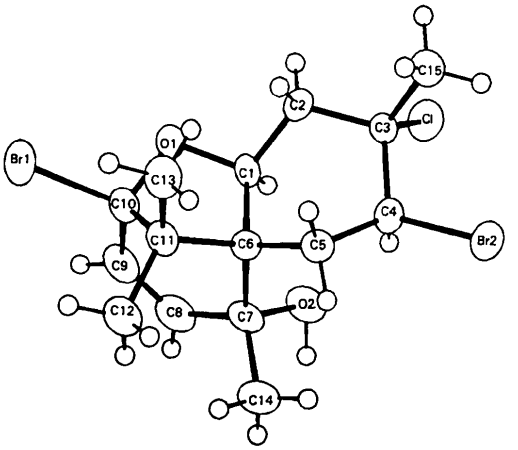

Fig. 1. Absolute configuration and standard sesquiterpene numbering scheme for title compound.

Related literature. Isolation from *Laurencia majuscula*: Caccamese, Compagnini & Toscano (1986). Original determination, as isolated from *Laurencia pacifica*: Sims, Fenical, Wing & Radlick (1971). Isolation from other *Laurencia* species: Sims, Fenical, Wing & Radlick (1973), Waraszkiewicz & Erickson (1974), Selover & Crews (1980), Suzuki (1980). Isolation from Californian mollusk *Aplysia*, which feeds on *Laurencia* species: Stallard & Faulkner (1974). Chemical constituents of *Laurencia* species: Erickson (1983), Faulkner (1984), Caccamese, Toscano, Cerrini & Gavuzzo (1982).

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Acta Cryst. (1986). C**42**, 1651–1652

Structure of Octahydro-2a*H*-azirino[1,2-*a*]indol-2a-ol

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(*Received* 3 *March* 1986; *accepted* 18 *June* 1986)

Abstract. $C_9H_{15}NO$, $M_r = 153{\cdot}2$, monoclinic, $P2_1/c$, $a = 10{\cdot}57\ (2)$, $b = 8{\cdot}93\ (1)$, $c = 9{\cdot}36\ (1)$ Å, $\beta = 105{\cdot}4\ (2)°$, $V = 851{\cdot}8$ Å^3, $Z = 4$, $D_x = 1{\cdot}20$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71073$ Å, $\mu = 0{\cdot}724$ cm^{-1}, $F(000) = 336$, $T = 294$ K, $R = 0{\cdot}059$ for 929 observed reflexions. The stereochemistry of the molecule has been established. Bond lengths: C–C in the three-membered ring, 1·460 Å; other C–C, 1·510–1·533 Å; C–N, 1·479–1·486 Å; C–O, 1·403 Å. Shortest intermolecular contact: O–H···N, 2·801 Å.

Experimental. Material prepared from 2-cyanohexahydroindolium salts by reduction with $LiAlH_4$ and hydrolysis with NaOH, white crystals (m.p. 402 K) from ether (Carlsson, Olesen & Lawesson, 1980). Crystal size 0·2 × 0·4 × 0·8 mm, space group and unit cell from photographs taken with Cu and Mo radiations. Data collection on a computer-controlled Supper diffractometer (Weissenberg geometry) with graphite-monochromated Mo $K\alpha$ radiation, a scintillation counter and a pulse-height analyser. 2484 independent reflexions were measured by the background–peak–background method out to $\sin\theta = 0{\cdot}5$, $-14 \le h \le 14$, $0 \le k \le 12$, $0 \le l \le 13$. Standard reflexion 202 monitored every 25 reflexions, ±4% variation; data rescaled to correct for this. 929 reflexions with $I > 3\sigma(I)$ were used in the refinement. No correction was applied for absorption. Structure solved with *MULTAN* (Germain, Main & Woolfson, 1971). Coordinates, anisotropic thermal parameters

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Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($\times 10^3$) *with e.s.d.'s in parentheses*

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$. The e.s.d. for U_{eq} is the mean of those for the diagonal elements of U_{ij}.

	x	y	z	U_{eq}(Å^2)
O	1142 (3)	11606 (3)	5605 (3)	42 (2)
N	433 (3)	9692 (3)	6984 (3)	33 (2)
C(1)	2387 (4)	11136 (4)	8104 (4)	40 (2)
C(2)	3793 (5)	11478 (7)	8105 (6)	61 (3)
C(3)	4476 (5)	10245 (8)	7495 (6)	73 (4)
C(4)	3660 (5)	9773 (7)	5963 (6)	63 (3)
C(5)	2305 (4)	9250 (4)	6049 (5)	43 (2)
C(6)	1568 (3)	10459 (4)	6646 (4)	30 (2)
C(7)	−211 (4)	10561 (5)	7940 (5)	44 (2)
C(8)	799 (4)	9476 (5)	8637 (4)	42 (2)
C(9)	2176 (5)	10060 (5)	9288 (4)	48 (3)

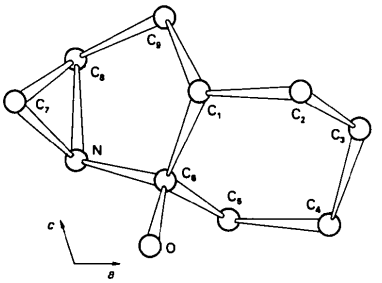

Fig. 1. Projection of the molecule showing the numbering of the atoms.

and a scale factor were refined by full-matrix least-squares calculations based on F and with unit weights. H atoms located on a difference map and included in refinement with isotropic thermal parameters. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Final $R = 0.059$ and $wR = 0.061$ for 100 parameters and 929 reflexions. $(\Delta/\sigma)_{max} = 0.4$, $\Delta\rho = -0.3$ to 0.4 e Å^{-3}. Fig. 1. is a projection of the molecule showing the numbering of the atoms, coordinates are listed in Table 1, bond

Table 2. *Bond lengths* (Å) *and angles* (°)

C(1)–C(2)	1·517 (7)	C(6)–O	1·403 (4)
C(1)–C(6)	1·533 (6)	C(6)–N	1·486 (5)
C(1)–C(9)	1·528 (6)	N–C(7)	1·479 (5)
C(2)–C(3)	1·510 (9)	N–C(8)	1·504 (5)
C(3)–C(4)	1·524 (8)	C(7)–C(8)	1·460 (7)
C(4)–C(5)	1·529 (7)	C(8)–C(9)	1·514 (6)
C(5)–C(6)	1·522 (5)		
C(2)–C(1)–C(6)	113·7 (4)	N–C(6)–C(5)	105·8 (3)
C(2)–C(1)–C(9)	117·3 (4)	C(1)–C(6)–C(5)	112·5 (4)
C(6)–C(1)–C(9)	103·9 (3)	C(6)–N–C(7)	114·5 (3)
C(1)–C(2)–C(3)	114·8 (5)	C(6)–N–C(8)	106·0 (3)
C(2)–C(3)–C(4)	110·5 (5)	C(7)–N–C(8)	58·6 (3)
C(3)–C(4)–C(5)	109·8 (5)	N–C(7)–C(8)	61·6 (3)
C(4)–C(5)–C(6)	112·4 (4)	N–C(8)–C(7)	59·9 (3)
O–C(6)–N	110·8 (3)	N–C(8)–C(9)	109·1 (3)
O–C(6)–C(1)	109·4 (3)	C(7)–C(8)–C(9)	117·5 (4)
O–C(6)–C(5)	111·3 (3)	C(1)–C(9)–C(8)	103·4 (4)
N–C(6)–C(1)	106·8 (3)		

distances and angles are given in Table 2.* Computer programs used: *DATAP* and *DSORTH* (State University of New York, Buffalo) – data processing; modified *ORFLS* (Busing, Martin & Levy, 1962) – least-squares refinement; *ORTEP* (Johnson, 1965) – bonds and angles.

* Lists of structure factors, anisotropic thermal parameters and coordinates for H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43156 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1986). C**42**, 1652–1654

Structure of 5,6-Dimethylbenzimidazole

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(*Received* 25 *January* 1986; *accepted* 28 *May* 1986)

Abstract. $C_9H_{10}N_2$, $M_r = 146.19$, monoclinic, $P2_1/c$, $a = 6.513$ (2), $b = 27.794$ (6), $c = 14.058$ (2) Å, $\beta = 102.62$ (2)°, $V = 2483.3$ Å^3, $Z = 12$, $D_m = 1.17$, $D_x = 1.173$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 0.67$ cm^{-1}, $F(000) = 936$, $T = 298$ K, final $R = 0.045$ for 2962 observed reflections. There are three crystal-

0108-2701/86/111652-03$01.50