and four ethylenediammonium groups, which are also independent. Of these four organic groups two are centrosymmetric.

As shown in Fig. 1, a projection along the *c* axis, the structure can be easily described as a set of rows parallel to the *c* axis. The first kind of row consists of alternating P_3O_9 and ethylenediammonium groups. These rows are arranged in an almost regular hexagonal way to give large hexagonal channels, which are centered by rows of ethylenediammonium groups. Main interatomic distances and bond angles in the P_3O_9 ring anions and the organic groups are reported in Table 2.

The three-dimensional network of hydrogen bonds, connecting the H atoms of the NH_3 radicals to the external O atoms of the phosphoric ring anions, is also detailed in Table 2.

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A New Indole Alkaloid from *Aristotelia chilensis*

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Abstract. 4,4-Dimethyl-8-methylene-3-azabicyclo[3.3.1]non-2-en-2-yl 3-indolyl ketone (1), $C_{20}H_{22}N_2O$, $M_r = 306{\cdot}41$, orthorhombic, $P2_12_12_1$, $a = 6{\cdot}480\ (1)$, $b = 12{\cdot}844\ (2)$, $c = 19{\cdot}960\ (3)$ Å, $V = 1661{\cdot}3\ (4)$ Å^3, $Z = 4$, $D_x = 1{\cdot}225$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}71$ cm^{-1}, $F(000) = 656$, $T = 293$ K, $R = 0{\cdot}0498$ for 923 reflections. The indole portion of the molecule is planar (0·018 Å r.m.s.d.). The heterocyclic six-membered ring exhibits a 1,2-diplanar conformation while the cyclohexane ring is in a chair conformation. The carbonyl group is almost coplanar with the indole system but the planar portion of the heterocyclic six-membered ring is twisted out of the indole plane by 47·4 (7)°.

Introduction. Members of the genus *Aristotelia* (Eleocarpaceae) are of interest because of the taxonomic problems they present (Allan, 1961) and because they produce a number of unique and interesting alkaloids. *Aristotelia peduncularis* Hook, collected in Tasmania, yielded peduncularine (2) plus three unidentified components (Bick, Bremner, Preston & Calder, 1971). *Aristotelia serrata* from New Zealand contains peduncularine (2), aristoteline (3) and several unidentified components (Anderson, Robertson, Avey, Donovan, Bick, Bremner, Finney, Preston, Gallagher & Russell, 1975). *Aristotelia chilensis,* collected in Chile, has yielded aristoteline (3), aristotelinine (4) (Gopalakrishna, Watson, Silva & Bittner, 1978), aristotelone (5) (Bhakuni, Silva, Matlin & Sammes, 1976), and aristone (6) (Bittner, Silva, Gopalakrishna, Watson, Zabel, Matlin & Sammes, 1978). Compound (6) was postulated to arise *via* rearrangement of a derivative of (4) (Zabel, Watson, Bittner & Silva, 1980). A reinvestigation of *A. chilensis* yielded two new isomeric indole alkaloids of unknown structure which differ only in the posi-

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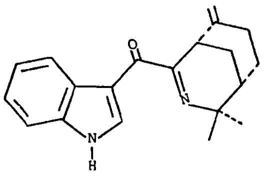
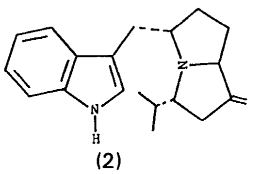
tion of a double bond. A single crystal of (1) was obtained and found suitable for X-ray diffraction studies. In compound (1), the double bond at C(5)—C(16) is exocyclic while in the isomer NMR data indicate it is shifted to C(5)—C(12). In principle, (1) can be visualized as arising from (3) or a derivative of (3) by breaking the C(5)—C(5*a*) bond.



(1)



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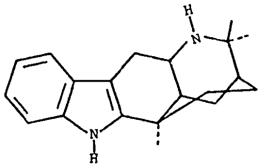

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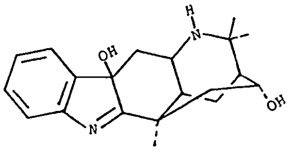
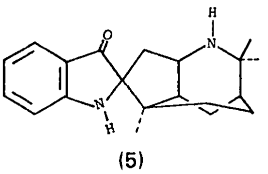
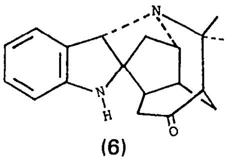


(4)



(5)



(6)

Table 1. *Atomic coordinates* (× 10^4) *and equivalent isotropic thermal parameters* (Å^2 × 10^3)

	x	*y*	*z*	U_{eq}*
N(1)	7544 (7)	−426 (3)	6114 (2)	43 (1)
C(2)	7995 (8)	−1554 (4)	6233 (3)	46 (2)
C(3)	7550 (9)	−1946 (4)	6946 (3)	56 (2)
C(4)	5578 (8)	−1457 (4)	7198 (3)	55 (2)
C(4*a*)	5948 (8)	−270 (4)	7240 (3)	47 (2)
C(5)	7640 (9)	−34 (4)	7742 (3)	57 (2)
C(5*a*)	9836 (7)	1566 (4)	6005 (3)	46 (2)
N(6)	10903 (7)	2344 (3)	5717 (2)	51 (2)
C(6*a*)	9612 (8)	3186 (4)	5614 (2)	42 (2)
C(7)	10048 (9)	4142 (4)	5314 (3)	53 (2)
C(8)	8459 (9)	4843 (4)	5281 (3)	58 (2)
C(9)	6537 (9)	4622 (4)	5552 (3)	57 (2)
C(10)	6117 (8)	3673 (4)	5844 (3)	48 (2)
C(10*a*)	7680 (7)	2931 (4)	5875 (2)	35 (2)
C(10*b*)	7830 (7)	1874 (3)	6116 (2)	38 (2)
O(11)	4463 (5)	1583 (3)	6514 (2)	62 (2)
C(11)	6201 (9)	1241 (4)	6401 (2)	42 (2)
C(11*a*)	6649 (7)	112 (4)	6564 (2)	38 (2)
C(12)	9487 (11)	−617 (6)	7669 (4)	98 (3)
C(13)	9241 (9)	−1746 (5)	7480 (3)	73 (2)
C(14)	6657 (11)	−2138 (4)	5724 (3)	85 (3)
C(15)	10247 (9)	−1664 (4)	6024 (3)	74 (3)
C(16)	7389 (14)	694 (5)	8219 (3)	94 (3)

* Equivalent isotropic *U* defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table 2. *Bond distances* (Å) *and valence angles* (°)

N(1)—C(2)	1·496 (6)	N(1)—C(11*a*)	1·272 (6)
C(2)—C(3)	1·536 (8)	C(2)—C(14)	1·532 (8)
C(2)—C(15)	1·524 (8)	C(3)—C(4)	1·510 (8)
C(3)—C(13)	1·550 (8)	C(4)—C(4*a*)	1·546 (7)
C(4*a*)—C(5)	1·516 (8)	C(4*a*)—C(11*a*)	1·507 (7)
C(5)—C(12)	1·419 (9)	C(5)—C(16)	1·345 (8)
C(5*a*)—N(6)	1·344 (7)	C(5*a*)—C(10*b*)	1·377 (7)
N(6)—C(6*a*)	1·383 (6)	C(6*a*)—C(7)	1·396 (7)
C(6*a*)—C(10*a*)	1·395 (7)	C(7)—C(8)	1·369 (8)
C(8)—C(9)	1·387 (8)	C(9)—C(10)	1·378 (7)
C(10)—C(10*a*)	1·391 (7)	C(10*a*)—C(10*b*)	1·444 (6)
C(10*b*)—C(11)	1·449 (7)	O(11)—C(11)	1·229 (7)
C(11)—C(11*a*)	1·515 (7)	C(12)—C(13)	1·508 (10)
C(2)—N(1)—C(11*a*)	120·1 (4)	N(1)—C(2)—C(3)	115·3 (4)
N(1)—C(2)—C(14)	104·9 (4)	C(3)—C(2)—C(14)	110·3 (4)
N(1)—C(2)—C(15)	103·5 (4)	C(3)—C(2)—C(15)	113·8 (5)
C(14)—C(2)—C(15)	108·3 (5)	C(2)—C(3)—C(4)	109·4 (4)
C(2)—C(3)—C(13)	116·7 (5)	C(4)—C(3)—C(13)	107·5 (5)
C(3)—C(4)—C(4*a*)	107·2 (4)	C(4)—C(4*a*)—C(5)	110·2 (4)
C(4)—C(4*a*)—C(11*a*)	108·6 (4)	C(5)—C(4*a*)—C(11*a*)	108·0 (4)
C(4*a*)—C(5)—C(12)	115·9 (5)	C(4*a*)—C(5)—C(16)	121·3 (6)
C(12)—C(5)—C(16)	122·8 (6)	N(6)—C(5*a*)—C(10*b*)	109·9 (4)
C(5*a*)—N(6)—C(6*a*)	109·5 (4)	N(6)—C(6*a*)—C(7)	129·0 (5)
N(6)—C(6*a*)—C(10*a*)	107·7 (4)	C(7)—C(6*a*)—C(10*a*)	123·3 (5)
C(6*a*)—C(7)—C(8)	116·5 (5)	C(7)—C(8)—C(9)	121·5 (5)
C(8)—C(9)—C(10)	121·5 (5)	C(9)—C(10)—C(10*a*)	118·7 (5)
C(6*a*)—C(10*a*)—C(10)	118·4 (4)	C(6*a*)—C(10*a*)—C(10*b*)	106·5 (4)
C(10)—C(10*a*)—C(10*b*)	135·0 (4)	C(5*a*)—C(10*b*)—C(10*a*)	106·3 (4)
C(5*a*)—C(10*b*)—C(11)	126·1 (4)	C(10*a*)—C(10*b*)—C(11)	127·5 (4)
C(10*b*)—C(11)—O(11)	122·6 (4)	C(10*b*)—C(11)—C(11*a*)	118·8 (4)
O(11)—C(11)—C(11*a*)	118·6 (4)	N(1)—C(11*a*)—C(4*a*)	126·4 (4)
N(1)—C(11*a*)—C(11)	117·1 (4)	C(4*a*)—C(11*a*)—C(11)	116·5 (4)
C(5)—C(12)—C(13)	116·4 (6)	C(3)—C(13)—C(12)	114·0 (5)

Experimental. A colorless crystal of dimensions 0·15 × 0·18 × 0·45 mm was mounted on a Nicolet $R3m/\mu$ update of a $P2_1$ diffractometer; data collected in the ω-scan mode ($3 \leq 2\theta \leq 45°$), scan rate 4 to 29·3° min^{-1}, graphite-monochromated Mo $K\alpha$ radiation; lattice parameters from a least-squares refinement of 25 reflections ($22{\cdot}38 \leq 2\theta \leq 33{\cdot}27°$); systematic absences ($h00$, $h = 2n + 1$; $0k0$, $k = 2n + 1$; $00l$, $l = 2n + 1$) and Laue symmetry *mmm* consistent with space group $P2_12_12_1$; monitored reflections (025 and $1\bar{1}5$) showed only statistical variations in intensities; 1288 independent reflections measured ($h = 0,6$; $k = 0,13$; $l = 0,21$), $923 \geq 3\sigma(I)$; Lorentz–polarization corrections applied, ψ-scan empirical absorption correction (transmission factors 0·926 to 0·954); structure solved by direct methods, block-cascade least-squares refinement, H atoms located in difference map but were allowed to ride at fixed distances from attached atoms, isotropic thermal parameters were refined for three groupings of H atoms; $R = 0{\cdot}0498$ and $wR = 0{\cdot}0502$ for 211 parameters and 923 reflections (0·0797 and 0·0592 for all reflections), $S = 1{\cdot}017$; $(\Delta/\sigma)_{\max} = 0{\cdot}018$; largest peaks in the final difference map $+0{\cdot}17$ and $-0{\cdot}18$ e Å^{-3}; $\sum w(|F_o| - |F_c|)^2$ minimized with $w = [\sigma^2(F_o) + 0{\cdot}00087F_o^2]^{-1}$. All computer programs supplied by Nicolet for Desktop 30 Microeclipse and Nova 4/C configuration (Nicolet Instrument Corporation, 1986); atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). Table 1 lists atomic positional parameters and

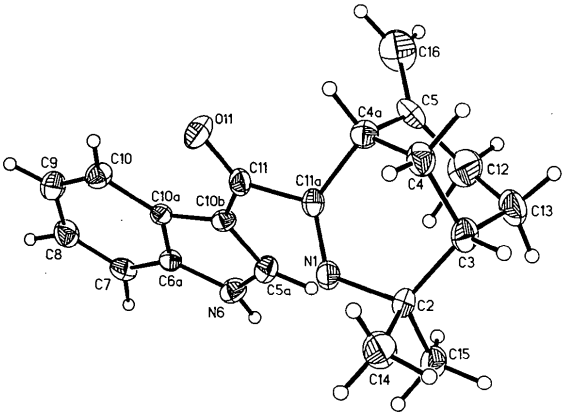


Fig. 1. Drawing of compound (1) with thermal ellipsoids at the 25% probability level. H atoms are represented by spheres of arbitrary size.

Table 2 interatomic distances and valence angles.* Fig. 1 is a thermal-ellipsoid drawing of (1).

Discussion. The indole portion of the molecule is planar (0·018 Å r.m.s.d.), and the N atom exhibits sp^2 hybridization. There is considerable delocalization in the five-membered ring with the C(5*a*)—C(10*b*) double bond elongated to 1·377 (7) Å, the two N(6)—C(sp^2) bonds of 1·344 (7) and 1·383 (6) Å and C(10*a*)—C(10*b*) = 1·444 (6) Å. The carbonyl group is almost coplanar with the indole moiety with C(11)—C(10*b*) = 1·449 (6) Å but not with the π system of the heterocyclic ring which is twisted 47·4 (7)° out of the plane resulting in C(11)—C(11*a*) = 1·515 (7) Å. The C(5*a*)—C(10*b*) bond is equivalent to the average value of the distances around the phenyl ring. The cyclohexane ring is in a slightly flattened chair conformation due to the C(5)—C(16) double bond. *cis* fusion and a double bond lead to a 1,2-diplanar conformation for the heterocyclic six-membered ring. The bond lengths and angles in this portion of the molecule are normal. There are only two intermolecular contacts less than 2·5 Å.

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* Lists of H-atom coordinates, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51872 (12 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of (20*R*)-20,21-Epoxy-19-norpregna-1,3,5(10)-triene-3,17β-diol

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Abstract. $C_{20}H_{26}O_3$, $M_r = 314{\cdot}4$, orthorhombic, $P2_12_12_1$, $a = 10{\cdot}25\ (1)$, $b = 25{\cdot}36\ (2)$, $c = 13{\cdot}11\ (1)$ Å, $V = 3410{\cdot}14$ Å^3, $Z = 8$, $D_x = 1{\cdot}225$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}45$ cm^{-1}, $F(000) = 1352$, $T = 293$ K. The structure was solved by direct methods and refined to $R = 0{\cdot}051$ for 2384 reflections with $F/\sigma(F) > 5$. Both the crystallographically independent molecules are in one 20*R* configuration

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