Fig. 3. Torsion angles of (a) Bixon & Lifson (1967) for cyclo-heptane and (b) the title compound. Deviations (Å) of atoms from a plane through the cycloheptane(ene) ring are also shown.

given in Table 3 with the deviations of individual atoms from this plane.

The arrangement of the molecules in the unit cell is shown in Fig. 2. The structure is stabilized by a three-dimensional network of hydrogen bonds of $N-H\cdots Br$ and $O-H\cdots Br$ types. Three of the four protons available for the hydrogen bonding take part in hydrogen bonding of the former type and the fourth in that of the latter. The hydrogen-bond lengths and angles are given in Table 4. The torsion angles around various bonds of the heptene ring shown in Fig. 3 agree closely with those of Bixon & Lifson (1967) for the chair conformation.

The author wishes to express his thanks to Professor R. Srinivasan for helpful discussions and constant encouragement.

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The Optically Active Form of the Alkaloid Jamine

By Joann K. Frank, Eileen N. Duesler, Nina N. Thayer,
Roland Heckendorn, Kenneth L. Rinehart Jr and Iain C. Paul*

Department of Chemistry, University of Illinois, Urbana, Illinois 61801, USA

and Renuka Misra

Department of Chemistry, University of Toronto, Toronto, Ontario, Canada

Abstract. $C_{21}H_{35}N_3$, $M_r = 329\cdot5$, orthorhombic, $a = 6\cdot367$ (3), $b = 12\cdot730$ (7), $c = 23\cdot106$ (8) Å, $Z = 4$, $P2_12_12_1$. The X-ray analysis ($R = 0\cdot055$ on 1315 reflections) of an alkaloid obtained from Ormosia costulata showed it to be the optically active form of jamine which has previously been reported as a race-mate.
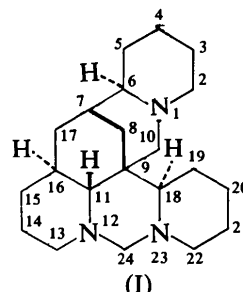
Introduction. In the course of an extended investigation of the Ormosia genus, a large number of alkaloids have been isolated from numerous species of this genus (Rinehart et al., 1978). In particular, an alkaloid, $[\alpha]_D^{26} = -8\cdot7°$ (c 1·0 g/100 ml, $CHCl_3$), was obtained from Ormosia costulata and was crystallized from acetone to give colorless crystals (m.p. 120–122°C). The same compound was isolated during an investigation of the alkaloidal extract of the bark of

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* Author to whom correspondence should be addressed.

Podopetalum ormondii F. Muell (McLean & Misra, 1978) by treatment of one of the fractions isolated with formaldehyde–formic acid to give a formaldehyde adduct, m.p. 126–127°C (from acetone, undepressed in mixture melting point with the *O. costulata* alkaloid), $[\alpha]_D^{24} = -10.4°$ (*c* 1·2 g/100 ml, CHCl$_3$).

The cell constants of the crystals from *O. costulata*, given in the *Abstract*, and the intensity data were obtained on a Picker FACS-1 diffractometer (Cu $K\alpha$, $\lambda = 1.54178$ Å). A 2θ scan was used with the backgrounds being collected at each limit of the scan for a period of 10 s. 1315 of the 1917 measured reflections ($2\theta < 130°$) were judged to be significant at the 2σ level. The structure was determined using the *MULTAN* direct-methods program (Germain, Main & Woolfson, 1971) and has been refined to final agreement factors for the non-zero reflections of $R = 0.055$ and $R_w = 0.047$ [$R_w = (\sum w\|F_{obs}| - |F_{calc}\|^2 / \sum w|F_{obs}|^2)^{1/2}$]. The final value of $|\sum w(|F_{obs}| - |F_{calc}|)^2/(m - n)]^{1/2}$, where m is the number of independent observations and n is the number of

variables, is 2·04.* The weighting scheme described by Corfield, Doedens & Ibers (1967) was used and the scattering curves were those compiled by Cromer & Mann (1968), except that for H (Stewart, Davidson & Simpson, 1965). The atomic coordinates are listed in Table 1.
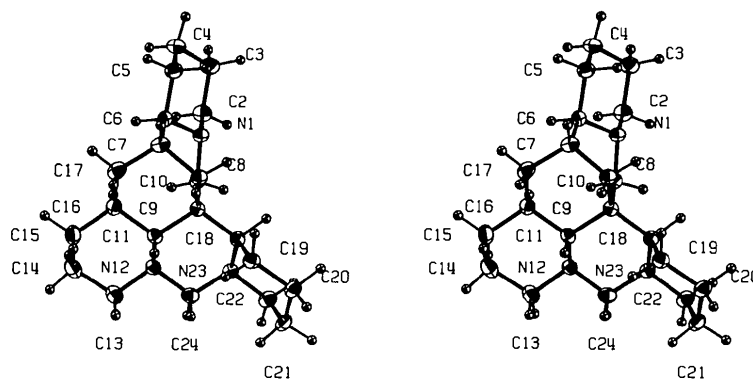

(I)

Fig. 1. Stereoscopic view of a single molecule of the optically active form of jamine.
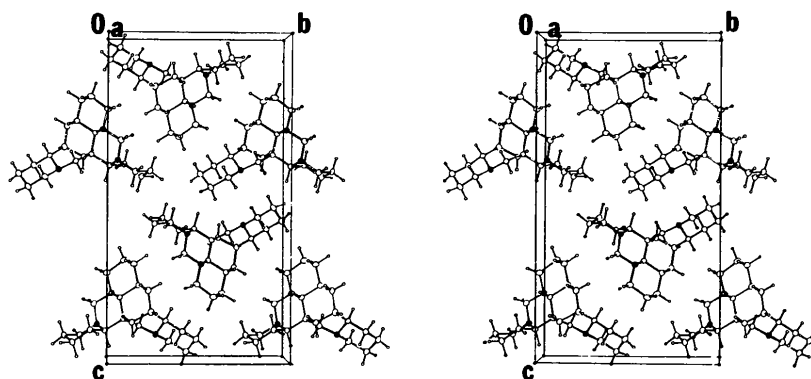

Fig. 2. Stereoscopic view of the packing of molecules of (I). The reference molecule has the darker bonds. All the N atoms are shown as full circles.

Table 1. *Final atomic coordinates for* (I) *in fractions of the unit-cell edge*

	x	y	z
N(1)	0·7849 (6)	0·7670 (3)	0·5852 (2)
C(2)	0·6301 (9)	0·8412 (5)	0·5617 (3)
C(3)	0·7390 (11)	0·9336 (5)	0·5316 (3)
C(4)	0·8919 (10)	0·9871 (5)	0·5727 (3)
C(5)	1·0405 (10)	0·9072 (4)	0·5985 (2)
C(6)	0·9187 (8)	0·8183 (4)	0·6284 (2)
C(7)	1·0712 (8)	0·7386 (4)	0·6566 (2)
C(8)	1·0562 (10)	0·6323 (4)	0·6264 (2)
C(9)	0·8302 (8)	0·5905 (4)	0·6327 (2)
C(10)	0·6739 (8)	0·6745 (4)	0·6095 (2)
C(11)	0·7928 (8)	0·5697 (4)	0·6976 (2)
N(12)	0·5828 (7)	0·5247 (3)	0·7070 (2)
C(13)	0·5492 (12)	0·4994 (5)	0·7681 (2)
C(14)	0·5743 (13)	0·5947 (5)	0·8067 (3)
C(15)	0·7884 (12)	0·6453 (5)	0·7976 (3)
C(16)	0·8184 (9)	0·6706 (4)	0·7337 (2)
C(17)	1·0288 (11)	0·7227 (5)	0·7211 (2)
C(18)	0·7981 (9)	0·4892 (4)	0·5977 (2)
C(19)	0·9757 (9)	0·4073 (4)	0·6025 (2)
C(20)	0·9267 (11)	0·3122 (4)	0·5650 (3)
C(21)	0·7115 (10)	0·2658 (5)	0·5816 (3)
C(22)	0·5432 (10)	0·3503 (4)	0·5786 (3)
N(23)	0·5894 (6)	0·4452 (3)	0·6126 (2)
C(24)	0·5610 (10)	0·4275 (4)	0·6741 (2)
H(2A)	0·541 (8)	0·871 (4)	0·593 (2)
H(2B)	0·540 (8)	0·804 (4)	0·531 (2)
H(3A)	0·826 (8)	0·907 (4)	0·495 (2)
H(3B)	0·638 (7)	0·990 (4)	0·518 (2)
H(4A)	0·817 (7)	1·020 (3)	0·603 (2)
H(4B)	0·979 (6)	1·036 (3)	0·550 (2)
H(5A)	1·131 (7)	0·870 (4)	0·562 (2)
H(5B)	1·136 (8)	0·942 (3)	0·630 (2)
H(6)	0·832 (7)	0·852 (3)	0·662 (2)
H(7)	1·211 (7)	0·764 (3)	0·653 (2)
H(8A)	1·085 (7)	0·639 (3)	0·586 (2)
H(8B)	1·159 (7)	0·586 (3)	0·645 (2)
H(10A)	0·567 (8)	0·698 (3)	0·639 (2)
H(10B)	0·584 (8)	0·643 (3)	0·576 (2)
H(11)	0·898 (6)	0·519 (3)	0·713 (1)
H(13A)	0·656 (8)	0·439 (4)	0·782 (2)
H(13B)	0·404 (8)	0·469 (4)	0·771 (2)
H(14A)	0·563 (10)	0·568 (4)	0·846 (2)
H(14B)	0·470 (7)	0·643 (3)	0·801 (2)
H(15A)	0·784 (8)	0·716 (4)	0·822 (2)
H(15B)	0·895 (7)	0·599 (3)	0·808 (2)
H(16)	0·704 (6)	0·715 (3)	0·724 (1)
H(17A)	1·038 (7)	0·788 (3)	0·741 (2)
H(17B)	1·134 (7)	0·678 (4)	0·738 (2)
H(18)	0·796 (7)	0·512 (3)	0·551 (2)
H(19A)	1·000 (7)	0·392 (3)	0·644 (2)
H(19B)	1·115 (7)	0·450 (3)	0·593 (2)
H(20A)	0·929 (10)	0·335 (4)	0·520 (3)
H(20B)	1·036 (7)	0·250 (4)	0·565 (2)
H(21A)	0·724 (8)	0·241 (3)	0·622 (2)
H(21B)	0·681 (8)	0·204 (4)	0·555 (2)
H(22A)	0·523 (8)	0·367 (4)	0·536 (2)
H(22B)	0·388 (8)	0·318 (4)	0·590 (2)
H(24A)	0·664 (7)	0·369 (3)	0·690 (2)
H(24B)	0·408 (8)	0·401 (3)	0·682 (2)

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

The C—H bond lengths range from 0·91 (5) to 1·12 (5) Å.

N(1)—C(2)	1·469 (7)		C(11)—C(16)	1·540 (7)
N(1)—C(6)	1·467 (6)		N(12)—C(13)	1·464 (7)
N(1)—C(10)	1·484 (6)		N(12)—C(24)	1·458 (7)
C(2)—C(3)	1·533 (9)		C(13)—C(14)	1·514 (9)
C(3)—C(4)	1·521 (9)		C(14)—C(15)	1·522 (11)
C(4)—C(5)	1·512 (9)		C(15)—C(16)	1·523 (8)
C(5)—C(6)	1·536 (8)		C(16)—C(17)	1·523 (9)
C(6)—C(7)	1·548 (7)		C(18)—C(19)	1·542 (8)
C(7)—C(8)	1·525 (9)		C(18)—N(23)	1·482 (7)
C(7)—C(17)	1·529 (8)		C(19)—C(20)	1·520 (8)
C(8)—C(9)	1·541 (8)		C(20)—C(21)	1·541 (9)
C(9)—C(10)	1·556 (7)		C(21)—C(22)	1·520 (8)
C(9)—C(11)	1·541 (7)		C(22)—N(23)	1·470 (7)
C(9)—C(18)	1·535 (7)		N(23)—C(24)	1·450 (7)
C(11)—N(12)	1·471 (7)			

C(2)—N(1)—C(6)	110·7 (4)		N(12)—C(11)—C(16)	110·0 (4)
C(2)—N(1)—C(10)	109·3 (4)		C(11)—N(12)—C(13)	111·1 (4)
C(6)—N(1)—C(10)	111·8 (4)		C(11)—N(12)—C(24)	109·9 (4)
N(1)—C(2)—C(3)	110·9 (5)		C(13)—N(12)—C(24)	107·6 (4)
C(2)—C(3)—C(4)	110·5 (5)		N(12)—C(13)—C(14)	112·1 (5)
C(3)—C(4)—C(5)	110·2 (5)		C(13)—C(14)—C(15)	110·6 (6)
C(4)—C(5)—C(6)	110·9 (5)		C(14)—C(15)—C(16)	109·6 (5)
N(1)—C(6)—C(5)	108·3 (4)		C(11)—C(16)—C(17)	110·7 (4)
N(1)—C(6)—C(7)	111·0 (4)		C(11)—C(16)—C(15)	109·6 (4)
C(5)—C(6)—C(7)	110·8 (4)		C(15)—C(16)—C(17)	112·8 (5)
C(6)—C(7)—C(8)	110·5 (4)		C(7)—C(17)—C(16)	113·5 (5)
C(6)—C(7)—C(17)	112·7 (4)		C(9)—C(18)—C(19)	115·7 (4)
C(8)—C(7)—C(17)	108·5 (5)		C(9)—C(18)—N(23)	108·3 (4)
C(7)—C(8)—C(9)	108·8 (4)		C(19)—C(18)—N(23)	112·7 (4)
C(8)—C(9)—C(10)	109·1 (4)		C(18)—C(19)—C(20)	110·3 (5)
C(8)—C(9)—C(11)	107·2 (4)		C(19)—C(20)—C(21)	110·3 (5)
C(8)—C(9)—C(18)	111·4 (4)		C(20)—C(21)—C(22)	110·1 (5)
C(10)—C(9)—C(11)	110·7 (4)		C(21)—C(22)—N(23)	114·6 (5)
C(10)—C(9)—C(18)	108·1 (4)		C(18)—N(23)—C(22)	111·5 (4)
C(11)—C(9)—C(18)	110·3 (4)		C(18)—N(23)—C(24)	113·5 (4)
N(1)—C(10)—C(9)	111·8 (4)		C(22)—N(23)—C(24)	111·8 (4)
C(9)—C(11)—C(16)	111·6 (4)		N(12)—C(24)—N(23)	111·5 (4)
C(9)—C(11)—N(12)	110·5 (4)			

Fig. 1. The absolute configuration was not determined and is not implied in (I) or the figures. The bond lengths and angles are listed in Table 2. It is of particular interest that the molecular structure is identical to that for jamine, an alkaloid that has been isolated in an optically inactive form from *Ormosia panamensis* and *Ormosia jamaicensis* (Naegeli, Wildman & Lloyd, 1963). The crystal and molecular structure of jamine was reported by Karle & Karle (1964), but as the racemate in space group P1. The melting point of the racemate was 153–154 °C, while that of the optically active form was 126–127 °C. The conformations of the rings are very similar in the two structures, with the N(1),C(6)–C(10) ring being in the boat conformation and all others in the chair conformation. The bond lengths and angles are consistent with generally accepted values and with those found for homo-dasycarpine (Wang, Duesler, Thayer, Heckendorn, Rinehart & Paul, 1978). The packing of molecules in

Discussion. The structural formula is shown in (I) and a stereoscopic view of a single molecule, together with the atom numbering used in the analysis, is given in

the present structure is shown in Fig. 2. The shortest intermolecular distances are 3·73 Å between C(22) in the reference molecule and C(19) in the molecule at $(-1 + x, y, z)$, and 3·74 Å between C(21) in the reference molecule and C(4) in the molecule at $(x, -1 + y, z)$.

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Homodasycarpine, an *Ormosia* Alkaloid

BY ANDREW H.-J. WANG, EILEEN N. DUESLER, NINA N. THAYER, ROLAND HECKENDORN, KENNETH L. RINEHART JR AND IAIN C. PAUL*

Department of Chemistry, University of Illinois, Urbana, Illinois 61801, USA

Abstract. $C_{21}H_{35}N_3$, $M_r = 329·5$, orthorhombic, $a = 6·835$ (1), $b = 9·243$ (1), $c = 29·420$ (2) Å, $Z = 4$, space group $P2_12_12_1$. The X-ray analysis ($R = 0·045$ on 1631 reflections) of the alkaloid, homodasycarpine, isolated from *Ormosia costulata* shows it to be a geometrical isomer of jamine.

Introduction. During an investigation of the alkaloids from numerous species of the *Ormosia* genus (Rinehart et al., 1978), an alkaloid, homodasycarpine, m.p. 130–140°C, $[\alpha]_D^{24} = +16 \pm 2°$ (CHCl$_3$) (Clarke & Grundon, 1963), was isolated from *Ormosia costulata* and crystallized from hexane–methylene dichloride. The cell constants and intensity data for the colorless crystals were obtained on a Picker FACS-1 diffractometer (Cu $K\bar{\alpha}$, $\lambda = 1·54178$ Å). Intensity data were collected using the 2θ scan with backgrounds being measured for 10 s at each limit of the scan. 1633 out of 1852 measured reflections ($2\theta < 130°$) were judged to be significant at the 2σ level. The structure was determined using the *MULTAN* direct-methods program

(Germain, Main & Woolfson, 1971) and has been refined to the final agreement factors of $R = 0·045$ and $R_w = 0·051$ $[R_w = (\sum w||F_{obs}| - |F_{calc}||^2/\sum w|F_{obs}|^2)^{1/2}]$. The final value of $[\sum w(|F_{obs}| - |F_{calc}|)^2/(m - n)]^{1/2}$, where m is the number of independent observations and n is the number of variables, is 3·01. The weighting scheme was that proposed by Corfield, Doedens & Ibers (1967), and the scattering curves for the non-hydrogen atoms were those compiled by Cromer & Mann (1968) and for H that by Stewart, Davidson & Simpson (1965). The atomic coordinates are listed in Table 1.†

Discussion. A stereoscopic view of a single molecule of homodasycarpine (I) is shown in Fig. 1, which also contains the atom numbering used in the analysis. The absolute configuration of the molecule was not established in this study and no implication of absolute con-

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* Author to whom correspondence should be addressed.

† Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33394 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.