

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

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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, $[\alpha]_D^{24} = +16 \pm 2^\circ$ ($CHCl_3$) (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 $K\alpha$, $\lambda = 1.54178$ 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 ($2\theta < 130^\circ$) 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-

† 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.

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

	<i>x</i>	<i>y</i>	<i>z</i>		<i>x</i>	<i>y</i>	<i>z</i>
N(1)	0.1840 (4)	0.6090 (3)	0.33311 (7)	H(5A)	-0.307 (5)	0.606 (3)	0.3355 (9)
C(2)	0.2007 (6)	0.6908 (4)	0.29083 (10)	H(5B)	-0.179 (5)	0.478 (3)	0.3093 (10)
C(3)	0.0442 (6)	0.6550 (4)	0.25539 (11)	H(6)	-0.033 (5)	0.724 (3)	0.3617 (9)
C(4)	-0.1576 (6)	0.6773 (4)	0.27609 (12)	H(7)	-0.163 (4)	0.529 (3)	0.4054 (9)
C(5)	-0.1783 (5)	0.5861 (4)	0.31931 (11)	H(8A)	-0.044 (5)	0.333 (3)	0.3636 (10)
C(6)	-0.0120 (5)	0.6203 (3)	0.35293 (10)	H(8B)	0.019 (4)	0.313 (3)	0.4171 (9)
C(7)	-0.0277 (5)	0.5303 (3)	0.39669 (10)	H(10A)	0.399 (4)	0.471 (3)	0.3209 (9)
C(8)	0.0339 (5)	0.3735 (3)	0.38794 (10)	H(10B)	0.204 (5)	0.400 (3)	0.3035 (9)
C(9)	0.2493 (5)	0.3712 (3)	0.37318 (9)	H(11)	0.511 (4)	0.433 (3)	0.3994 (8)
C(10)	0.2642 (5)	0.4625 (3)	0.32951 (9)	H(13A)	0.637 (6)	0.380 (4)	0.4776 (12)
C(11)	0.3777 (5)	0.4288 (3)	0.41251 (10)	H(13B)	0.499 (5)	0.307 (4)	0.5096 (10)
N(12)	0.3663 (4)	0.3280 (3)	0.45135 (8)	H(14A)	0.291 (6)	0.506 (4)	0.5195 (11)
C(13)	0.4958 (7)	0.3758 (4)	0.48855 (11)	H(14B)	0.506 (5)	0.547 (4)	0.5309 (11)
C(14)	0.4285 (7)	0.5190 (4)	0.50761 (11)	H(15A)	0.584 (5)	0.652 (4)	0.4615 (10)
C(15)	0.4319 (6)	0.6318 (4)	0.46983 (11)	H(15B)	0.378 (5)	0.726 (4)	0.4810 (10)
C(16)	0.3143 (5)	0.5821 (3)	0.42815 (9)	H(16)	0.345 (4)	0.655 (3)	0.4035 (8)
C(17)	0.0946 (5)	0.5907 (4)	0.43602 (10)	H(17A)	0.056 (5)	0.689 (3)	0.4423 (10)
C(18)	0.3081 (5)	0.2136 (3)	0.36110 (9)	H(17B)	0.055 (5)	0.535 (3)	0.4669 (10)
C(19)	0.5024 (5)	0.1965 (3)	0.33481 (11)	H(18)	0.198 (4)	0.175 (3)	0.3410 (9)
C(20)	0.5412 (7)	0.0354 (4)	0.32486 (13)	H(19A)	0.609 (5)	0.241 (3)	0.3521 (10)
C(21)	0.5326 (7)	-0.0550 (4)	0.36814 (14)	H(19B)	0.496 (5)	0.249 (3)	0.3017 (10)
C(22)	0.3395 (6)	-0.0273 (3)	0.39283 (12)	H(20A)	0.669 (7)	0.021 (4)	0.3096 (13)
N(23)	0.3017 (4)	0.1261 (4)	0.40275 (8)	H(20B)	0.435 (6)	0.004 (4)	0.3019 (11)
C(24)	0.4300 (6)	0.1825 (4)	0.43803 (11)	H(21A)	0.542 (6)	-0.156 (4)	0.3612 (11)
H(2A)	0.184 (5)	0.801 (4)	0.2966 (10)	H(21B)	0.641 (5)	-0.038 (4)	0.3887 (10)
H(2B)	0.337 (5)	0.685 (3)	0.2780 (10)	H(22A)	0.337 (6)	-0.085 (4)	0.4236 (11)
H(3A)	0.062 (5)	0.717 (4)	0.2317 (11)	H(22B)	0.201 (6)	-0.065 (4)	0.3719 (11)
H(3B)	0.057 (5)	0.558 (4)	0.2474 (10)	H(24A)	0.568 (5)	0.192 (3)	0.4265 (9)
H(4A)	-0.170 (5)	0.779 (4)	0.2839 (10)	H(24B)	0.423 (4)	0.116 (3)	0.4650 (9)
H(4B)	-0.260 (5)	0.654 (3)	0.2545 (10)				

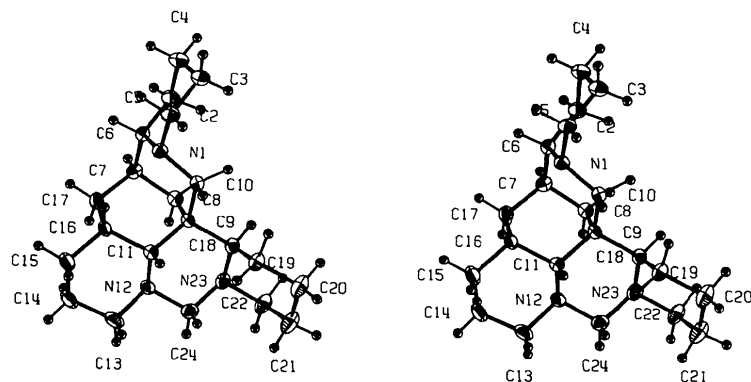


Fig. 1. A stereoscopic view of a single molecule of homodasyarpine.

figuration should be drawn from the figures. The bond lengths and angles are given in Table 2. The dimensions are in agreement with accepted values. The molecule of homodasyarpine can be seen to be a geometrical isomer of jamine (Karle & Karle, 1964; Frank, Duesler, Thayer, Heckendorn, Rinehart, Paul & Misra, 1978). The relative configurations of the two molecules are different at C(6), C(7), C(9), and C(16), with the result that in homodasyarpine all the six-membered rings are in the chair conformation. A stereoscopic view of the molecular packing is shown in

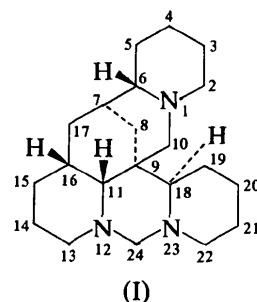


Table 2. Bond lengths (Å) and angles (°)

The C—H distances range from 0.89 (3) to 1.19 (4) Å.

N(1)—C(2)	1.460 (4)	C(11)—C(16)	1.551 (4)	N(1)—C(2)—C(3)	114.5 (3)	C(13)—N(12)—C(24)	107.1 (3)
N(1)—C(6)	1.465 (4)	N(12)—C(13)	1.475 (5)	C(2)—C(3)—C(4)	109.4 (3)	N(12)—C(13)—C(14)	110.8 (3)
N(1)—C(10)	1.465 (4)	N(12)—C(24)	1.466 (4)	C(3)—C(4)—C(5)	110.0 (3)	C(13)—C(14)—C(15)	108.9 (3)
C(2)—C(3)	1.530 (5)	C(13)—C(14)	1.509 (6)	C(4)—C(5)—C(6)	110.6 (3)	C(14)—C(15)—C(16)	111.7 (3)
C(3)—C(4)	1.522 (6)	C(14)—C(15)	1.524 (5)	N(1)—C(6)—C(5)	113.9 (3)	C(11)—C(16)—C(17)	111.6 (3)
C(4)—C(5)	1.532 (5)	C(15)—C(16)	1.537 (5)	N(1)—C(6)—C(7)	111.0 (2)	C(11)—C(16)—C(15)	111.3 (3)
C(5)—C(6)	1.540 (5)	C(16)—C(17)	1.521 (5)	C(5)—C(6)—C(7)	112.0 (3)	C(15)—C(16)—C(17)	112.3 (3)
C(6)—C(7)	1.537 (4)	C(18)—C(19)	1.545 (5)	C(6)—C(7)—C(8)	110.7 (3)	C(7)—C(17)—C(16)	113.9 (3)
C(7)—C(8)	1.531 (4)	C(18)—N(23)	1.469 (4)	C(6)—C(7)—C(17)	113.4 (3)	C(9)—C(18)—C(19)	115.7 (3)
C(7)—C(17)	1.533 (5)	C(19)—C(20)	1.540 (5)	C(8)—C(7)—C(17)	108.7 (3)	C(9)—C(18)—N(23)	108.5 (2)
C(8)—C(9)	1.535 (4)	C(20)—C(21)	1.524 (5)	C(7)—C(8)—C(9)	108.9 (2)	C(19)—C(18)—N(23)	112.8 (3)
C(9)—C(10)	1.540 (4)	C(21)—C(22)	1.528 (6)	C(8)—C(9)—C(10)	107.0 (2)	C(18)—C(19)—C(20)	110.0 (3)
C(9)—C(11)	1.547 (4)	C(22)—N(23)	1.471 (4)	C(8)—C(9)—C(11)	109.1 (2)	C(19)—C(20)—C(21)	111.4 (3)
C(9)—C(18)	1.553 (4)	N(23)—C(24)	1.456 (4)	C(8)—C(9)—C(18)	109.0 (2)	C(20)—C(21)—C(22)	109.8 (3)
C(11)—N(12)	1.476 (4)			C(10)—C(9)—C(11)	113.5 (2)	C(21)—C(22)—N(23)	114.1 (3)
				C(10)—C(9)—C(18)	107.8 (2)	C(18)—N(23)—C(22)	111.1 (3)
				C(11)—C(9)—C(18)	110.3 (2)	C(18)—N(23)—C(24)	112.3 (2)
C(2)—N(1)—C(6)	111.9 (2)	N(12)—C(11)—C(16)	109.4 (2)	N(1)—C(10)—C(9)	114.9 (2)	C(22)—N(23)—C(24)	112.4 (3)
C(2)—N(1)—C(10)	112.8 (2)	C(11)—N(12)—C(13)	110.7 (3)	C(9)—C(11)—C(16)	112.2 (2)	N(12)—C(24)—N(23)	109.9 (3)
C(6)—N(1)—C(10)	115.9 (2)	C(11)—N(12)—C(24)	110.9 (2)	C(9)—C(11)—N(12)	109.4 (2)		

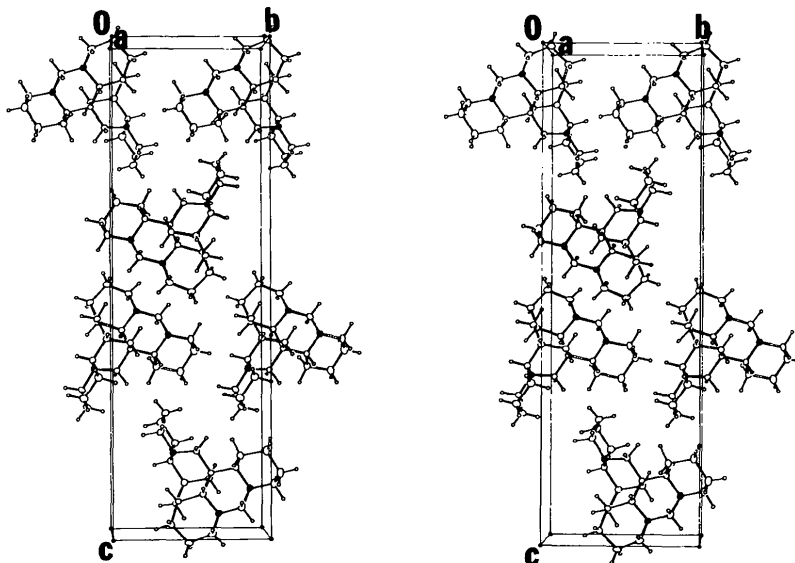


Fig. 2. Stereosopic view of the packing of molecules of (I). The reference molecule has the darker bonds. All the N atoms are shown as full circles.

Fig. 2. The shortest intermolecular contacts are 3.76 Å between C(16) in the reference molecule and C(22) in the molecule at $x, 1 + y, z$, and 3.62 and 3.71 Å between, respectively, N(12) and C(24) in the reference molecule and C(13) in the molecule at $-\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$.

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