after the deacetylation of (I), as already proposed (Hashimoto, Ohta, Shudo & Okamoto, 1979).

The estimated standard deviations of the bond lengths and angles are σ(C—C) = 0·007, σ(H—C) = 0·04 Å and σ(C—C—C) = 0·4, σ(C—C—H) = 2·5°. As is seen in Fig. 2, the C⩦C bond lengths range from 1·326 to 1·403 Å. The bond C(3)—C(14) produced by the reaction connects the two conjugated rings and is 1·481 Å, which is significantly shorter than the normal C—C single-bond length, but is comparable with those found in 1,1′-binaphthyl (1·475 Å, Kerr & Robertson, 1969).

The oxazine ring *B* takes a half-boat conformation; C(10) is displaced from the benzoxazine plane formed by C(12) ~ C(17), O(1) and N(1), by 0·394 (4) Å and C(11) is displaced by 0·138 (4) Å in the same direction. The dihedral angle between the two rings *A* and *C*, 57·5 (5)°, is intermediate between those found in 3,3′-difluorobiphenyl (44°) by photoelectron spectroscopy (Main & Turner, 1972), and in 1,1′-binaphthyl (68°, Kerr & Robertson, 1969). The *b*-axis projection of the crystal structure is shown in Fig. 3.

The indole rings are stacked along the diad screw axis with an interplanar distance of 3·193 (4) Å, forming a column of molecules. The molecules within a column are held together by hydrogen bonds from the indole N(2) to the methoxy O(3) [2·969 (5) Å]. The benzoxazine ring projects out from the column and interacts with that of the neighbouring column in pairs.

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9-Isopropyl-9,10-dihydroacridine

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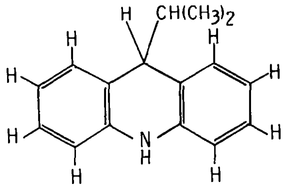
Abstract. $C_{16}H_{17}N$, monoclinic, $P2_1/n$, $Z = 4$, $M_r = 223{\cdot}31$, $a = 19{\cdot}937\,(2)$, $b = 5{\cdot}672\,(1)$, $c = 11{\cdot}140\,(1)$ Å, $\beta = 99{\cdot}75\,(1)°$, $V = 1241{\cdot}4\,(2)$ Å^3, $D_x = 1{\cdot}195$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ(Cu $K\alpha$) = 0·533 mm^{-1}; final $R = 0{\cdot}056$. The isopropyl group is in a 'quasi-axial' conformation with respect to the central ring. The folding angle between the best planes of the two benzene rings is 156·1°.

Introduction. Single crystals of the title compound (I) were obtained through the courtesy of Dr C. T. Taylor of the Chemistry Department of the University of Sheffield, Sheffield, England. The crystals are clear prisms elongated along the *b* axis. The unit-cell parameters were obtained from a least-squares analysis of 15 reflections with 2θ values in the range from 45 to 90°. The space group $P2_1/n$ was deduced from systematic absences (0*k*0 absent with *k* odd, *h*0*l* absent with *h* + *l* odd). The intensity data were collected on a Syntex $P2_1$ automatic diffractometer with a crystal approximately 0·15 × 0·66 × 0·21 mm with the *b* axis of the crystal along the φ axis of the diffractometer. A $\theta/2\theta$ scanning mode with graphite-monochromated Cu $K\alpha$ radiation was used to measure 1586 independent reflections with 2θ values below 130°, of which 1363 reflections were considered as observed by the criterion $I > 3{\cdot}0\sigma(I)$, where $\sigma(I)$ was determined from counting statistics. The intensity data were reduced to structure amplitudes by the application of Lorentz and



(I)

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polarization factors, and no absorption corrections were applied.

The structure was determined by the application of direct methods with the weighted multisolution tangent-refinement program *MULTAN* (Germain, Main & Woolfson, 1971). The E map showed the positions of all non-hydrogen atoms. The refinement was carried out by the full-matrix least-squares method (Busing, Martin & Levy, 1962) with isotropic temperature factors and the block-diagonal least-squares method (Shiono, 1971) with anisotropic temperature factors. Most of the H positions were located on a difference Fourier synthesis, and the rest were calculated with reasonable bond lengths and bond angles with respect to the atoms to which they are bonded. The isotropic temperature factors were used for the H atoms in the refinement. The weight of a reflection was assigned as $1/[\sigma(F)]^2$, where $\sigma(F)$ was calculated from counting statistics. The quantity $\sum w(|F_o| - |F_c|)^2$ was minimized. The final R index ($\sum ||F_o| - |F_c||/\sum |F_o|$) was 0·056,* and the weighted disagreement index, R_w, was 0·060. The magnitude $[\sum w(F_o - F_c)^2/(m-n)]^{1/2}$, was 0·99. The atomic scattering factors used for C and N atoms were those from *International Tables for X-ray Crystallography* (1962). For H, the values given by Stewart, Davidson & Simpson (1965) were used. The final positional parameters are given in Table 1.

Table 1. *Fractional atomic coordinates* ($\times 10^4$, *for* H $\times 10^3$) *and isotropic thermal parameters*

The estimated standard deviations are given in parentheses and refer to the last positions of respective values.

	x	y	z	B_{eq}/B (Å^2)*
N(10)	3256 (1)	5860 (3)	1454 (2)	3·74 (8)
C(1)	3756 (1)	806 (4)	−238 (2)	3·82 (10)
C(2)	3447 (1)	1344 (5)	−1420 (2)	4·33 (11)
C(3)	3095 (1)	3427 (5)	−1641 (2)	4·38 (11)
C(4)	3029 (1)	4934 (4)	−698 (2)	3·94 (10)
C(5)	3070 (1)	6183 (4)	3537 (2)	4·01 (10)
C(6)	3149 (1)	5298 (5)	4707 (2)	4·55 (11)
C(7)	3508 (1)	3245 (5)	4994 (2)	4·62 (11)
C(8)	3788 (1)	2092 (4)	4115 (2)	4·02 (10)
C(9)	4093 (1)	1803 (4)	1995 (2)	3·32 (8)
C(11)	3714 (1)	2298 (4)	725 (2)	3·22 (9)
C(12)	3333 (1)	4381 (4)	491 (2)	3·22 (8)
C(13)	3357 (1)	5024 (4)	2649 (2)	3·14 (8)
C(14)	3738 (1)	2974 (4)	2939 (2)	3·14 (8)
C(15)	4852 (1)	2527 (5)	2096 (2)	4·35 (11)
C(16)	5272 (1)	1770 (6)	3308 (3)	5·86 (14)
C(17)	4947 (1)	5128 (6)	1892 (3)	6·23 (15)
H(N)	300 (1)	690 (4)	128 (2)	5·0 (5)
H(1)	401 (1)	−61 (4)	−6 (2)	4·2 (5)
H(2)	350 (1)	23 (4)	−205 (2)	4·7 (5)
H(3)	284 (1)	396 (4)	−246 (2)	4·6 (5)
H(4)	277 (1)	627 (4)	−84 (2)	3·7 (5)
H(5)	282 (1)	747 (4)	330 (2)	4·5 (5)
H(6)	291 (1)	593 (4)	525 (2)	4·7 (5)
H(7)	354 (1)	251 (4)	580 (2)	5·3 (5)
H(8)	402 (1)	59 (4)	435 (2)	4·3 (5)
H(9)	408 (1)	15 (4)	212 (2)	3·4 (5)
H(15)	501 (1)	155 (4)	138 (2)	4·3 (5)
H(16)1	521 (1)	19 (4)	342 (2)	5·4 (5)
H(16)2	517 (1)	285 (4)	403 (2)	4·8 (5)
H(16)3	575 (1)	171 (4)	332 (2)	5·2 (5)
H(17)1	474 (1)	548 (4)	114 (2)	5·0 (5)
H(17)2	480 (1)	580 (4)	255 (2)	4·8 (5)
H(17)3	541 (1)	535 (4)	203 (2)	5·1 (5)

* B_{eq} is calculated from the relation

$$B_{eq} = \tfrac{1}{3} \textstyle\sum_i \sum_j B_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j.$$

Discussion. The crystal structure of 9-isopropyl-9,10-dihydroacridine is one of a series of tricyclic compounds under study in this laboratory. The conformations of a number of dihydroacridine derivatives in solution have been studied by the NMR technique (Taylor & Procter, 1971). The objectives of the present study are to determine the conformation in the solid state and to compare the conformation with that obtained in solution. The identification of the atoms and the configuration of the molecule are shown in Fig. 1. The conformation of the central ring is intermediate between a boat and a half-boat, and the ring torsion angles are also shown in Fig. 1. The Cremer & Pople (1975) puckering parameters for the central ring are $q_2 = 0{\cdot}321$, $q_3 = 0{\cdot}050$, $Q = 0{\cdot}326$ Å, $\varphi_2 = 180{\cdot}3$ and $\theta = 79{\cdot}5°$. This conformation is similar to that in 9-*tert*-butyl-9,10-dihydroacridine (Chu & Rosenstein, 1979). The isopropyl group is in a 'quasi-axial' conformation as compared to the 'axial' conformation of the *tert*-butyl group in 9-*tert*-butyl-9,10-dihydroacridine. The torsion angles C(11)–C(9)–C(15)–C(16), C(11)–C(9)–C(15)–C(17), C(14)–C(9)–C(15)–C(16), and C(14)–C(9)–C(15)–C(17) are −172·7 (2), 62·3 (3), 62·9 (3), and −62·1 (3)°, respectively. The conformation of the isopropyl substituent with respect to the central ring in the title

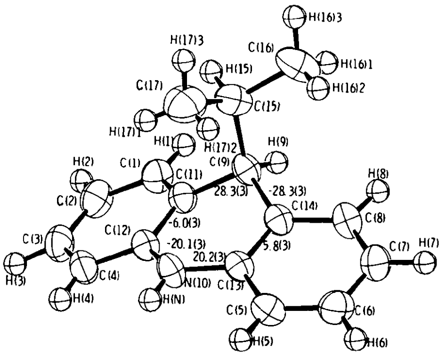

Fig. 1. *ORTEP* drawing (Johnson, 1965) of one molecule of the title compound with torsion angles (°) around the central ring.

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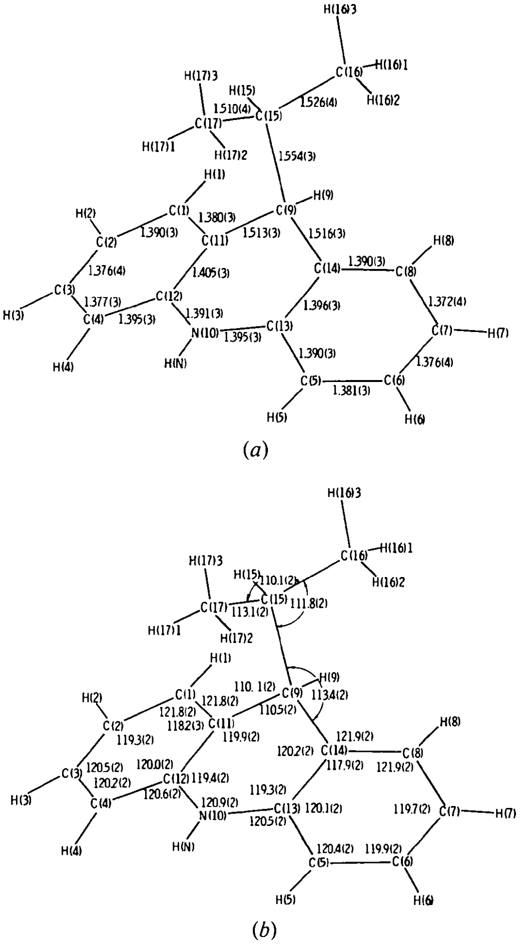
* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35417 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

compound is similar to that in *N*-isopropylphenothiazine (Chu & van der Helm, 1976) and 9-isopropylxanthene (Chu & Yang, 1977). The 'axial' conformation of the 9-isopropyl substituent was also predicted by NMR (Taylor & Procter, 1971) in solution.

The bond lengths and bond angles with their standard deviations are shown in Fig. 2. The mean value of the C—N bond length is 1·393 (3) Å, and the C—N—C bond angle is 120·9 (2)°. The C—N bond length in the title compound is 0·02 Å shorter than that in 9-*tert*-butyl-9,10-dihydroacridine (Chu & Rosenstein, 1979); however, the C—N—C bond angle is the same for both dihydroacridines. The value of the C(9)—C(15) bond length of 1·554 (3) Å is also the same for both dihydroacridines. The C—H bond lengths range from 0·90 to 1·06 Å (mean 0·96 ± 0·02 Å) and N—H is 0·79 (2) Å. The C—C—H bond angles involving benzene rings range from 114 to 125° (mean 120 ± 1°) and C—C—H and H—C—H involving tetrahedral C atoms range from 97 to 120° (mean 109 ± 1°). The mean value of the two C—N—H bond angles is 116 (2)°. The packing of the molecules in the crystal is shown in Fig. 3. There are no intermolecular contacts less than van der Waals distances.



(*a*)

(*b*)

Fig. 2. (*a*) Bond lengths (Å) and (*b*) bond angles (°) of the title compound with e.s.d.'s in parentheses.

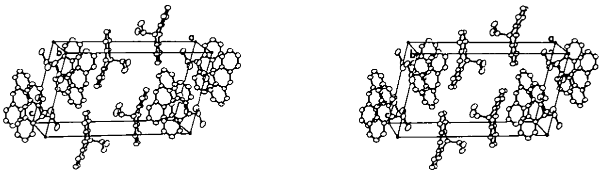


Fig. 3. The molecular packing of the title compound in a unit cell.

The equations of the least-squares planes of the two benzene rings are $0{\cdot}8683x + 0{\cdot}4740y - 0{\cdot}2914z = 6{\cdot}799$ and $0{\cdot}8053x + 0{\cdot}5340y + 0{\cdot}1175z = 7{\cdot}269$ (where x, y, and z are in Å) for rings *A* and *B* (Fig. 1) respectively. The deviations of atoms from the planes range from 0·001 to 0·019 Å. The folding angle between the planes of the two benzene rings is 156·1°, compared with 150·2° in 9-*tert*-butyl-9,10-dihydroacridine (Chu & Rosenstein, 1979).

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