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

The estimated standard deviations of the bond 
lengths and angles are $\sigma$(C–C) = 0.007, $\sigma$(H–C) = 
0.04 Å and $\sigma$(C–C–C) = 0.4, $\sigma$(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 (C3)–(C14) 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 spectros-
copy (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.

References

HASHIMOTO, Y., OHTA, T., SHUDO, K. & OKAMOTO, T. 
HASHIMOTO, Y., SHUDO, K., OKAMOTO, T., NAGAO, M., 
191–194.
pp. 1146–1149.
MULTAN. A System of Computer Programs for the 
Automatic Solution of Crystal Structures from X-ray 
Diffraction Data. Univs. of York, England, and Louvain, 
Belgium.
54, pp. 149–167.
OKAYA, Y. & ASHIDA, T. (1967). HBLS IV. The Universal 
Crystallographic Computing System (1), p. 65. The 
Crystallographic Society of Japan.


9-Isopropyl-9,10-dihydroacridine

BY SHIRLEY S. C. CHU, ROBERT D. ROSENSTEIN AND VERA NAPOLEONE

School of Engineering and Applied Science, Southern Methodist University, Dallas, Texas 75275, USA

(Received 5 May 1980; accepted 13 June 1980)

Abstract. C18H15N, monoclinic, $P2_1/n$, $Z = 4$, $M_r =$ 
223.31, $a = 19.937(2)$, $b = 5.672(1)$, $c = 
11.140(1)$ Å, $\beta = 99.75(1)$°, $V = 1241.4(2)$ Å³,
$D_x = 1.195$ Mg m–3, $\lambda$(Cu $K\alpha$) = 1.5418 Å, $\mu$(Cu $K\alpha$) = 0.533 mm–1; final $R = 0.056$. 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 (0k0 absent with k odd, h0l 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 
θ/2θ 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 
$I > 3.0\sigma(I)$, where $\sigma(I)$ was determined from counting 
statistics. The intensity data were reduced to structure 
amplitudes by the application of Lorentz and
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

<table>
<thead>
<tr>
<th></th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>$B_{eq}/\AA^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>N(10)</td>
<td>3256</td>
<td>5860</td>
<td>1454</td>
<td>3.74 (8)</td>
</tr>
<tr>
<td>C(1)</td>
<td>3756</td>
<td>806</td>
<td>-238</td>
<td>3.82 (10)</td>
</tr>
<tr>
<td>C(2)</td>
<td>3447</td>
<td>1344</td>
<td>-1420</td>
<td>4.33 (11)</td>
</tr>
<tr>
<td>C(3)</td>
<td>3095</td>
<td>3427</td>
<td>-1641</td>
<td>4.38 (11)</td>
</tr>
<tr>
<td>C(4)</td>
<td>3029</td>
<td>4934</td>
<td>-698</td>
<td>3.94 (10)</td>
</tr>
<tr>
<td>C(5)</td>
<td>3070</td>
<td>6183</td>
<td>3537</td>
<td>4.01 (10)</td>
</tr>
<tr>
<td>C(6)</td>
<td>3149</td>
<td>5298</td>
<td>4707</td>
<td>4.55 (11)</td>
</tr>
<tr>
<td>C(7)</td>
<td>3508</td>
<td>3245</td>
<td>4994</td>
<td>4.62 (11)</td>
</tr>
<tr>
<td>C(8)</td>
<td>3788</td>
<td>2092</td>
<td>4115</td>
<td>4.02 (10)</td>
</tr>
<tr>
<td>C(9)</td>
<td>4093</td>
<td>1803</td>
<td>1995</td>
<td>3.32 (8)</td>
</tr>
<tr>
<td>C(11)</td>
<td>3714</td>
<td>2298</td>
<td>725</td>
<td>3.22 (9)</td>
</tr>
<tr>
<td>C(12)</td>
<td>3333</td>
<td>4381</td>
<td>491</td>
<td>3.22 (8)</td>
</tr>
<tr>
<td>C(13)</td>
<td>3557</td>
<td>5024</td>
<td>2649</td>
<td>3.14 (8)</td>
</tr>
<tr>
<td>C(14)</td>
<td>3738</td>
<td>2974</td>
<td>2939</td>
<td>3.14 (8)</td>
</tr>
<tr>
<td>C(15)</td>
<td>4852</td>
<td>2527</td>
<td>2096</td>
<td>4.35 (11)</td>
</tr>
<tr>
<td>C(16)</td>
<td>5272</td>
<td>1770</td>
<td>3308</td>
<td>5.86 (14)</td>
</tr>
<tr>
<td>C(17)</td>
<td>4947</td>
<td>5128</td>
<td>1892</td>
<td>6.23 (15)</td>
</tr>
<tr>
<td>H(N)</td>
<td>300</td>
<td>690</td>
<td>128</td>
<td>5.0 (5)</td>
</tr>
<tr>
<td>H(1)</td>
<td>401</td>
<td>-61</td>
<td>-6</td>
<td>2.5 (5)</td>
</tr>
<tr>
<td>H(2)</td>
<td>350</td>
<td>234</td>
<td>-205</td>
<td>4.7 (5)</td>
</tr>
<tr>
<td>H(3)</td>
<td>284</td>
<td>396</td>
<td>-246</td>
<td>4.6 (5)</td>
</tr>
<tr>
<td>H(4)</td>
<td>277</td>
<td>627</td>
<td>-84</td>
<td>3.7 (5)</td>
</tr>
<tr>
<td>H(5)</td>
<td>282</td>
<td>747</td>
<td>330</td>
<td>4.5 (5)</td>
</tr>
<tr>
<td>H(6)</td>
<td>291</td>
<td>593</td>
<td>525</td>
<td>4.5 (5)</td>
</tr>
<tr>
<td>H(7)</td>
<td>354</td>
<td>251</td>
<td>380</td>
<td>5.3 (5)</td>
</tr>
<tr>
<td>H(8)</td>
<td>401</td>
<td>59</td>
<td>435</td>
<td>4.3 (5)</td>
</tr>
<tr>
<td>H(9)</td>
<td>408</td>
<td>15</td>
<td>212</td>
<td>3.4 (5)</td>
</tr>
<tr>
<td>H(10)</td>
<td>501</td>
<td>155</td>
<td>138</td>
<td>4.3 (5)</td>
</tr>
<tr>
<td>H(11)</td>
<td>521</td>
<td>19</td>
<td>342</td>
<td>5.4 (5)</td>
</tr>
<tr>
<td>H(12)</td>
<td>517</td>
<td>285</td>
<td>403</td>
<td>4.8 (5)</td>
</tr>
<tr>
<td>H(13)</td>
<td>575</td>
<td>171</td>
<td>332</td>
<td>5.2 (5)</td>
</tr>
<tr>
<td>H(14)</td>
<td>474</td>
<td>548</td>
<td>114</td>
<td>5.0 (5)</td>
</tr>
<tr>
<td>H(15)</td>
<td>480</td>
<td>580</td>
<td>255</td>
<td>4.8 (5)</td>
</tr>
<tr>
<td>H(16)</td>
<td>541</td>
<td>535</td>
<td>203</td>
<td>5.1 (5)</td>
</tr>
</tbody>
</table>

* $B_{eq}$ is calculated from the relation $B_{eq} = \frac{1}{\sum \sum_j \sum_j B_{ij} \sigma_i \sigma_j a_i a_j}$.

**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 $q_2 = 0.321$, $q_3 = 0.050$, $Q = 0.326$, $\phi_2 = 180.8$ and $\theta = 79.5^\circ$. 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 $C(11)-C(9)-C(15)-C(17)$, $C(11)-C(9)-C(15)-C(17)$, $C(14)-C(9)-C(15)-C(17)$, and $C(14)-C(9)-C(15)-C(17)$ are $-172.7 (2)$, $62.3 (3)$, $62.9 (3)$, and $-62.1 (3)^\circ$, respectively. The conformation of the isopropyl substituent with respect to the central ring in the title compound with torsion angles ($\phi$) around the central ring.

Fig. 1. ORTEP drawing (Johnson, 1965) of one molecule of the title compound with torsion angles ($\phi$) around the central ring.
9-ISOPROPYL-9,10-DIHYDROACRIDINE

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—H bond angle is the same for both dihydroacridines. 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.

The equations of the least-squares planes of the two benzene rings are 0.8683x + 0.4740y - 0.2914z = 6.799 and 0.8053x + 0.5340y + 0.1175z = 7.269 (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).

This research was supported by the Robert A. Welch Foundation, Houston, Texas. The authors wish to thank Dr C. A. Taylor of the University of Sheffield, England, for kindly supplying the crystals and Dr R. Shiono of the University of Pittsburgh for making the ORTEP plots.

References
