benzenoid fragments amount to 0·010 (2), 0·011 (3) and 0·014 (2) Å for rings *A*, *B* and *D*, respectively.

Both fluorenyl systems are significantly nonplanar: the dihedral angle between the least-squares planes through rings *A* and *B* is 172·2 (2)°, while that between the planes of rings *C* and *D* amounts to 168·1 (2)°. We may confidently ascribe this conformational feature to intramolecular effects, since there are only two intermolecular contacts shorter by 0·1 Å or more than the sum of van der Waals radii (C 1·7, H 1·2 Å); they are: C(5′)···C(5′) (at $-x$, $-y$, $1-z$), 3·281 (3), and H(6′)···H(153) (at x, $1+y$, z), 2·23 (2) Å.

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Structure of 7-Methoxy-6-(2-methyl-3-indolyl)-2*H*-1,4-benzoxazin-3(4*H*)-one

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Abstract. $C_{18}H_{16}N_2O_3$, monoclinic, space group $P2_1/a$, $a = 20{\cdot}182$ (10), $b = 7{\cdot}323$ (4), $c = 10{\cdot}656$ (5) Å, $\beta = 90{\cdot}74$ (1)°, $Z = 4$. The final R value is 0·08 including H atoms. The compound is obtained by an unusual reaction of 4-acetoxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one with 2-methylindole and the present study has established its structure.

Introduction. Derivatives of 4-hydroxybenzoxazine found in graminaceous plants (Hofman & Hofmanoa', 1969) as biologically active substances (Hashimoto, Shudo, Okamoto, Nagao, Takahashi & Sugimura, 1978) have some quite novel reactivities and several unexpected reaction products are obtained (Hashimoto, Ohta, Shudo & Okamoto, 1979). The present paper describes the X-ray diffraction study of a product obtained by an unusual reaction of 4-acetoxy-7-methoxybenzoxazine with 2-methylindole [Fig. 1(III)].

The lattice constants and intensity data were obtained on a Philips PW 1100 diffractometer using graphite-monochromated Cu $K\alpha$ radiation by the θ–2θ scan method. The scans were repeated twice when the total counts during the first scan were less than 2000. The background was measured at each end of the scan range for half the total scan time. A total of 2389 reflexions were measured within the 2θ angle of 130°. Intensities were corrected for Lorentz and polarization

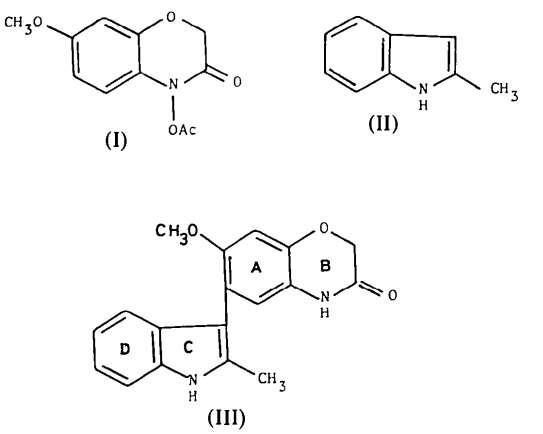

Fig. 1. The chemical structures of 4-acetoxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one (I), 2-methylindole (II) and 7-methoxy-6-(2-methyl-3-indolyl)-2*H*-1,4-benzoxazin-3(4*H*)-one (III).

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factors and averaged for the symmetry-equivalent reflexions, but no absorption correction was applied.

The crystal structure was determined by the direct method using *MULTAN* (Main, Woolfson & Germain, 1971) and refined by the block-diagonal least-squares method using *HBLS* IV (Okaya & Ashida, 1967). The final R value was 0·079 including H atoms. The final atomic coordinates are listed in Table 1.*

Discussion. The bond lengths and angles are shown in Fig. 2. The values are in good agreement with those of the related compounds benzoxazine (Søtofte, 1973) and indole (Hanson, 1964).

* Lists of structure factors and anisotropic temperature factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35392 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates* ($\times 10^4$ *for non-hydrogen atoms and* $\times 10^3$ *for hydrogen atoms*)

Estimated standard deviations are given in parentheses.

	x	y	z	$B_{eq.}$ (Å^2)
C(1)	3737 (2)	3567 (7)	5217 (5)	4·19 (0·08)
C(2)	3042 (2)	3715 (6)	5550 (4)	2·89 (0·06)
C(3)	2802 (2)	4148 (6)	6660 (4)	2·99 (0·06)
C(4)	2076 (2)	4085 (6)	6439 (4)	3·59 (0·06)
C(5)	1562 (2)	4324 (7)	7173 (4)	5·25 (0·08)
C(6)	899 (3)	4047 (8)	6637 (5)	6·87 (0·09)
C(7)	753 (3)	3579 (7)	5358 (6)	4·61 (0·09)
C(8)	1247 (3)	3374 (7)	4599 (5)	3·18 (0·08)
C(9)	1914 (2)	3601 (6)	5148 (4)	3·10 (0·07)
C(10)	4716 (3)	3706 (8)	11967 (4)	4·58 (0·09)
C(11)	4890 (2)	2131 (7)	11172 (4)	3·98 (0·08)
C(12)	4073 (2)	3381 (6)	9539 (4)	3·38 (0·06)
C(13)	3677 (2)	3136 (6)	8377 (4)	3·09 (0·06)
C(14)	3219 (2)	4475 (6)	7892 (4)	2·99 (0·06)
C(15)	3175 (2)	6068 (6)	8597 (4)	3·33 (0·06)
C(16)	3569 (2)	6317 (6)	9767 (4)	3·06 (0·07)
C(17)	4014 (2)	4943 (7)	10210 (4)	2·92 (0·07)
C(18)	2621 (3)	8936 (8)	8803 (5)	5·77 (0·10)
N(1)	4545 (2)	2028 (6)	9996 (3)	4·07 (0·06)
N(2)	2498 (2)	3420 (5)	4636 (3)	3·05 (0·06)
O(1)	4422 (2)	5249 (5)	11339 (3)	3·64 (0·06)
O(2)	5302 (2)	978 (5)	11591 (3)	5·26 (0·06)
O(3)	2730 (2)	7367 (4)	8078 (3)	4·36 (0·05)
H(C1)	382 (2)	239 (6)	502 (4)	5·23 (1·12)
H′(C1)	407 (2)	433 (6)	590 (4)	5·31 (1·12)
H″(C1)	386 (2)	416 (7)	432 (4)	5·59 (1·15)
H(C5)	165 (2)	467 (6)	806 (4)	4·30 (1·00)
H(C6)	48 (2)	419 (6)	720 (4)	4·47 (1·03)
H(C7)	23 (2)	332 (7)	502 (4)	5·90 (1·23)
H(C8)	117 (2)	288 (7)	368 (4)	5·49 (1·15)
H(N2)	252 (2)	286 (6)	390 (4)	5·09 (1·11)
H(N1)	459 (2)	91 (6)	946 (4)	4·71 (1·05)
H(C13)	372 (2)	190 (6)	788 (4)	3·75 (0·94)
H(C18)	240 (2)	851 (7)	967 (4)	5·83 (1·21)
H′(C18)	230 (2)	965 (6)	833 (4)	5·38 (1·14)
H″(C18)	302 (2)	951 (7)	899 (4)	5·88 (1·21)
H(C16)	356 (2)	750 (6)	1031 (4)	4·77 (1·06)
H(C10)	430 (2)	318 (7)	1243 (4)	5·66 (1·17)
H′(C10)	508 (2)	401 (7)	1253 (4)	5·51 (1·15)

It is now clear that the present compound is produced by the reaction of 4-acetoxy-7-methoxy-2*H*-1,4-benzoxazin-3(4*H*)-one (I) with 2-methylindole (II) in methylene chloride in such a way that the aromatic carbon atom at the 3-position of 2-methylindole undergoes a nucleophilic attack on the 6-position of the benzoxazine derivative immediately

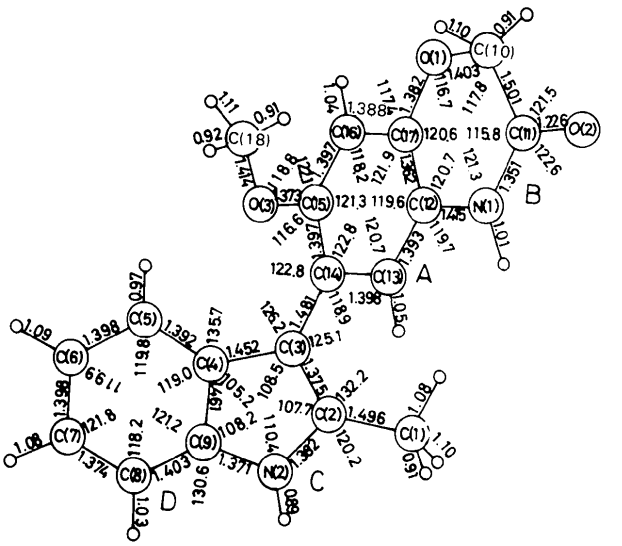

Fig. 2. Bond lengths (Å) and angles (°) of the title compound.

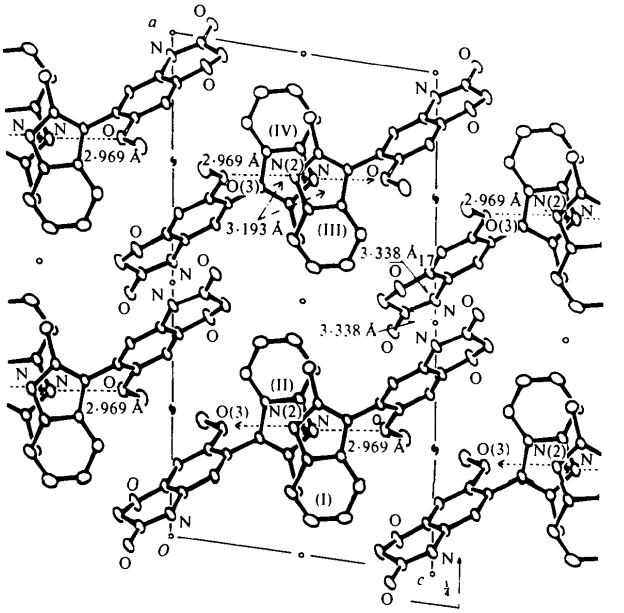

Fig. 3. Projection of the crystal structure along the *b* axis. Dashed lines indicate hydrogen bonds. The distance between the indole rings (*C* and *D* rings, and their symmetry-related planes) is denoted by a dot-dash line. Intermolecular short contacts between the benzoxazine rings are shown by dotted lines. Symmetry operations for the molecules are (I) x,y,z; (II) $\frac{1}{2}-x,\frac{1}{2}+y,1-z$; (III) $\frac{1}{2}+x,\frac{1}{2}-y,z$; (IV) $1-x,1-y,1-z$.

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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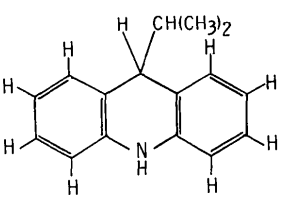
Abstract. $C_{16}H_{17}N$, monoclinic, $P2_1/n$, $Z = 4$, $M_r = 223{\cdot}31$, $a = 19{\cdot}937\ (2)$, $b = 5{\cdot}672\ (1)$, $c = 11{\cdot}140\ (1)$ Å, $\beta = 99{\cdot}75\ (1)°$, $V = 1241{\cdot}4\ (2)$ Å^3, $D_x = 1{\cdot}195$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ(Cu $K\alpha$) = 0·533 mm^{-1}; 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 Departmcnt 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 $\theta/2\theta$ 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



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