causes some shortening of the single bond C(19)—C(20) (Pauling, 1960).

The packing of the molecule viewed along **a** is shown in Fig. 2. The molecules are linked in chains by fairly strong hydrogen bonding between N(1)—H(N1)···O(2) [N(1)—H(N1) 1·040, N(1)···O(2) 3·122 (4), H(N1)···O(2) 2·19 Å, N(1)—H(N1)···O(2) 148·2°]. Parallel chains of hydrogen-bonded picrinine molecules are laterally displaced at regular intervals along the **c** direction. The hydrogen bonds together with the van der Waals forces associated with the other atoms represent the intermolecular interactions that stabilize the structure.

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A DNA-Intercalating Compound Derived from 7*H*-Pyridocarbazole: the Structure of 10-Methoxy-2-Methyl-7*H*-pyrido[4,3-*c*]carbazolium Iodide

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Abstract. $C_{17}H_{15}N_2O^+.I^-$, $M_r = 390{\cdot}22$, monoclinic, $P2_1/c$, $a = 10{\cdot}017$ (2), $b = 8{\cdot}123$ (5), $c = 19{\cdot}074$ (4) Å, $\beta = 95{\cdot}86$ (2)°, $V = 1544$ (2) Å^3, $Z = 4$, $D_x = 1{\cdot}67$ g cm^{-3}, $\mu = 2{\cdot}10$ cm^{-1}, λ(Mo $K\alpha$) = 0·7107 Å, $F(000) = 768$, $R = 0{\cdot}04$ for 1236 unique reflections measured at 295 K. Dimensions of the ring system are similar to those found in 6*H*-pyridocarbazole analogues (ellipticine derivatives). The iodine ion and pyridocarbazolium system are linked by a hydrogen bond. The planar 7*H*-pyridocarbazole cations form stacks approximately parallel to **b**. Interactions between stacks occur by weak van der Waals forces.

Introduction. In the series of 6*H*-pyridocarbazoles, several compounds, mainly derivatives of ellipticines (5,11-dimethyl-6*H*-pyrido[3,4-*b*]carbazole), show pronounced antitumor activity (Le Pecq, Dat-Xuong, Gosse & Paoletti, 1974). Activity on human tumors has been reported for some derivatives (Paoletti, Le Pecq, Dat-Xuong, Juret, Garnier, Amiel & Rouesse, 1980). This activity is related to the DNA-binding properties of this planar aromatic system. The mechanism involved in this interaction is an intercalation between adjacent base pairs in the DNA. Such properties are also found in the series of 7*H*-pyridocarbazoles, but if these derivatives are able to intercalate in DNA (Lauga, Delbarre & Roques, 1981), they show weak or no antitumor activity (Pelaprat, Oberlin, Le Guen, Roques & Le Pecq, 1980). The present study was undertaken to obtain more stereochemical information on this new

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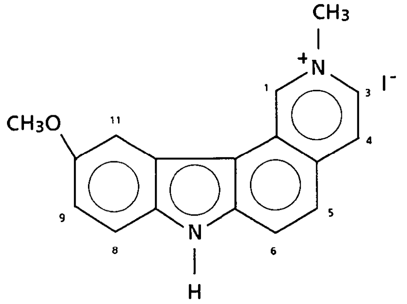
intercalating compound, as well as to compare it with the 6*H*-pyridocarbazole analogues in its interactions with DNA.



Experimental. Very small yellow crystals (needles) were obtained from methanol solution by vapor diffusion; crystal size 0·08 × 0·04 × 0·3 mm, X-ray precession photographs taken to determine crystal class and unit cell, accurate cell dimensions obtained by least-squares analysis on 24 reflections. Enraf–Nonius CAD-4 diffractometer, intensity collected with monochromated Mo $K\alpha$ radiation, ω–θ scans, width 1·9° + 0·35tanθ, intensities of three standard reflections monitored every 3 h, no crystal decomposition, $\theta_{\max} = 23°$, h(0 to 11), k(0 to 8), l(−21 to +21); 2265 unique reflections measured, 1236 observed reflections with $I \geq 2{\cdot}5\sigma(I)$. Lorentz–polarization corrections, no absorption corrections applied. Structure solution from a Patterson map, which revealed the I position, and subsequent Fourier maps. Block-diagonal least-squares refinement (on F) of non-H atoms with anisotropic thermal parameters and of H atoms with thermal parameters converged at $R = 0{\cdot}043$ and $wR = 0{\cdot}04$, with $w = 1/\sigma^2(F)$, highest peak in final difference Fourier map located near I atom, 0·5 e Å^{-3}, minimum height −0·4 e Å^{-3}, $(\Delta/\sigma)_{\max} = 0{\cdot}2$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974), all calculations performed on a BULL Mini 6-92 computer, local programs *CRISAFFI, CRISUTIL.*

Discussion. Final atomic parameters are in Table 1;* Fig. 1 shows a stereoview of the molecular structure; Table 2 gives the bond lengths and angles. E.s.d.'s are large, due in part to the ratio of variables to observations and to low crystal quality.

Comparison of the observed bond lengths with those of other 6*H*-pyridocarbazole derivatives (Courseille, Busetta & Hospital, 1974, 1981, 1982; Aggarwal,

Table 1. *Final atomic parameters and equivalent isotropic thermal parameters*

$$B_{\rm eq} = \tfrac{4}{3}\textstyle\sum_i\sum_j B_{ij}\mathbf{a}_i\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$(Å^2)
I(50)	−0·5736 (1)	0·1834 (1)	0·3689 (0)	5·6 (0)
C(1)	0·1993 (9)	0·2868 (13)	0·5178 (4)	3·5 (5)
N(2)	0·2844 (7)	0·2285 (9)	0·5710 (4)	3·8 (5)
C(3)	0·2399 (10)	0·1266 (12)	0·6202 (5)	4·2 (6)
C(4)	0·1099 (10)	0·0873 (13)	0·6197 (5)	4·2 (6)
C(5)	−0·1218 (10)	0·1108 (12)	0·5658 (5)	4·2 (6)
C(6)	−0·2104 (9)	0·1659 (13)	0·5139 (5)	4·2 (5)
N(7)	−0·2393 (7)	0·3318 (11)	0·4032 (4)	3·9 (4)
C(8)	−0·1844 (10)	0·5040 (13)	0·3008 (5)	4·5 (6)
C(9)	−0·0827 (10)	0·5763 (12)	0·2709 (5)	4·0 (6)
C(10)	0·0510 (10)	0·5570 (13)	0·3015 (5)	4·1 (6)
C(11)	0·0827 (9)	0·4730 (12)	0·3623 (5)	3·3 (5)
C(12)	−0·0220 (8)	0·3980 (11)	0·3949 (4)	2·7 (5)
C(13)	−0·0319 (8)	0·3061 (13)	0·4579 (4)	3·0 (5)
C(14)	0·0622 (8)	0·2482 (10)	0·5133 (5)	2·6 (5)
C(15)	0·0153 (9)	0·1470 (12)	0·5674 (5)	3·7 (6)
C(16)	−0·1668 (9)	0·2664 (11)	0·4605 (5)	3·6 (6)
C(17)	−0·1553 (9)	0·4180 (12)	0·3619 (5)	3·4 (5)
C(22)	0·4309 (8)	0·2750 (13)	0·5746 (5)	4·8 (6)
O(20)	0·1456 (7)	0·6368 (8)	0·2650 (3)	5·3 (4)
C(30)	0·2852 (9)	0·6316 (13)	0·2939 (5)	5·2 (7)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

C(1)–N(2)	1·34 (1)	C(8)–C(17)	1·37 (1)
C(1)–N(14)	1·40 (1)	C(9)–C(10)	1·41 (1)
N(2)–C(3)	1·36 (1)	C(10)–C(11)	1·36 (1)
C(3)–C(4)	1·34 (1)	C(10)–O(20)	1·39 (1)
C(4)–C(15)	1·39 (1)	C(11)–C(12)	1·41 (1)
C(5)–C(6)	1·34 (1)	C(12)–C(13)	1·43 (1)
C(5)–C(15)	1·40 (1)	C(12)–C(17)	1·43 (1)
C(6)–C(16)	1·41 (1)	C(13)–C(14)	1·42 (1)
N(7)–C(16)	1·36 (1)	C(13)–C(16)	1·40 (1)
N(7)–C(17)	1·40 (1)	C(14)–C(15)	1·44 (1)
C(8)–C(9)	1·35 (1)	O(20)–C(30)	1·45 (1)

N(2)–C(1)–C(14)	120·6 (8)	C(12)–C(13)–C(16)	107·5 (7)
C(1)–N(2)–C(3)	120·6 (7)	C(14)–C(13)–C(16)	117·9 (8)
N(2)–C(3)–C(4)	121·8 (8)	C(1)–C(14)–C(15)	118·3 (8)
C(3)–C(4)–C(15)	120·9 (9)	C(1)–C(4)–C(13)	122·8 (8)
C(5)–C(6)–C(16)	119·8 (9)	C(13)–C(14)–C(15)	118·9 (7)
C(16)–N(7)–C(17)	110·3 (7)	C(4)–C(15)–C(5)	122·6 (8)
C(9)–C(8)–C(17)	118·5 (9)	C(4)–C(15)–C(14)	117·8 (8)
C(8)–C(9)–C(10)	120·1 (9)	C(5)–C(15)–C(14)	119·7 (8)
C(9)–C(10)–C(11)	122·6 (9)	C(6)–C(16)–N(7)	129·0 (8)
C(9)–C(10)–O(20)	114·0 (8)	C(6)–C(16)–C(13)	122·2 (7)
C(11)–C(10)–O(20)	123·4 (8)	N(7)–C(16)–C(13)	108·8 (8)
C(10)–C(11)–C(12)	118·3 (8)	N(7)–C(17)–C(8)	130·5 (8)
C(11)–C(12)–C(13)	135·7 (8)	N(7)–C(17)–C(12)	106·5 (7)
C(11)–C(12)–C(17)	117·4 (8)	C(8)–C(17)–C(12)	123·0 (8)
C(13)–C(12)–C(17)	106·8 (7)	C(10)–O(20)–C(30)	118·4 (7)
C(12)–C(13)–C(14)	134·5 (8)		

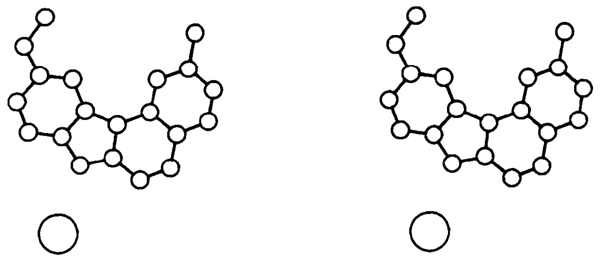


Fig. 1. Stereoview of the molecular structure.

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[*] Lists of structure factors, anisotropic temperature factors of the non-H atoms and coordinates of the H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51214 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

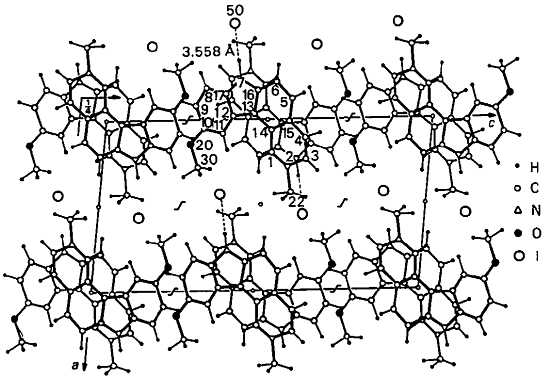

Fig. 2. Projection of the structure along **b**.

Neidle & Sainsbury, 1983) reveals virtually no significant differences. But a few C—C lengths are partially double bonded: C(6)—C(5), C(8)—C(9) and C(10)—C(11). The exocyclic angles around C(10) are markedly asymmetric. The four-fused-ring system is planar within experimental errors, as are ellipticine derivatives themselves. The methoxy group is placed nearly on the mean plane of the all-ring system whereas the I anion is outside the plane ($\delta = 0{\cdot}7$ Å) at 3·558 (7) Å from the N(7) atom and at 2·71 (7) Å from H(107). The distances are shorter than the sum of accepted van der Waals radii of N (1·60), I (2·15) and H (1·2 Å) atoms (Whuler, Brouty & Spinat, 1980; Nyburg & Faerman, 1985). The formation of a linear hydrogen bond N—H···I is also evidenced by the value 140 (5)° for the angle N(7)—H(107)···I. The most pronounced feature of the crystal structure is the alternating stacking (parallel to **b**) of two four-fused-ring systems related by a center of inversion (Fig. 2). A characteristic of the stacking mode is the prominent overlapping between the pyridine and benzene rings from both sides of the molecule. The ring separation is alternately 3·39 and 3·34 Å. Stacks are linked to I ions by the hydrogen bonds described above and to themselves by weak van der Waals forces.

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Structure de la Panarine Dihydratée, un Nouvel Alcaloïde Extrait d'un Curare Vénézuélien

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Abstract. Panarine dihydrate isolated from a kind of Venezuelan curare, $C_{20}H_{22}N_2O_2.2H_2O$, $M_r = 358{\cdot}44$, orthorhombic, $P2_12_12_1$, $a = 9{\cdot}125$ (5), $b = 13{\cdot}414$ (8), $c = 14{\cdot}953$ (7) Å, $V = 1830{\cdot}3$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}300$ g cm^{-3}, $\lambda(\text{Mo } K\bar{\alpha}) = 0{\cdot}7107$ Å, $\mu = 0{\cdot}53$ cm^{-1}, $T = 290$ K, $F(000) = 768$. Final $R = 0{\cdot}045$ for 2007 observed reflections. Structure solved by direct methods. Panarine has a conformation very similar to

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