The molecular conformation of (II) and the atom numbering appear in Fig. 1. Bond lengths and valency angles are given in Table 3, the different least-squares mean planes of the molecule are reported in Table 4.

The identification of the nitrogen atoms was based on chemical considerations. Their assignment is consistent with the shortest bonds and the location of all hydrogen atoms in the difference maps.

The relative orientation of the two aromatic systems, the aminophenyl and the isoquinoline, is given by the Newman projection along the C(2′)–C(7) bond, illustrated in Fig. 2.

The isoquinoline mean plane shows that several atoms of the ring deviate significantly from coplanarity: the molecule is slightly bent around the C(9)–C(10) bond, the dihedral angle between planes *A* and *B* being 1·1°.

A projection of the structure along **b**, illustrating the packing of molecules, is shown in Fig. 3. Molecules are linked into centrosymmetric dimers through weak hydrogen bonds involving the nitrogen of the amino group and the isoquinoline nitrogen [N(7′) $\cdots$N(2) = 3·28 Å; N(7′)–N$\cdots$N(2) = 162°].

We wish to thank Dr Claude Thal for suggesting the problem and for interesting discussions.

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Spiro[2*H*-indole-3,7′-(1′-methyl-6′-cyano-1′,8′,2′,3′-tetrahydro-7′*H*-1′-pyridine)]

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Abstract. $C_{17}H_{17}N_3$, $M=265·35$; monoclinic $P2_1/c$; $a=9·736$ (7), $b=11·791$ (12), $c=12·566$ (10) Å, $\beta=91·15$ (8)°, $V=1442·3$ Å^3; $Z=4$, $d_{calc}=1·22$ g cm^{-3}. The structure has been refined by full-matrix least-squares calculations to a final *R* value of 6·2% with 1156 observed intensities.

Table 1. *Final coordinates and thermal parameters* (× 10^4) *and their e.s.d.'s for the non-hydrogen atoms*

B is the equivalent isotropic thermal factor. The anisotropic thermal coefficients are in the form:

$$\exp\,[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)].$$

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B
N(1)	7981 (3)	3471 (2)	6507 (2)	109 (4)	57 (3)	104 (3)	−20 (3)	−30 (3)	−3 (2)	4·6
C(2)	7136 (3)	2766 (3)	7215 (3)	98 (4)	58 (3)	73 (3)	8 (3)	−20 (3)	−27 (2)	3·9
C(3)	6783 (3)	1683 (2)	6564 (3)	75 (4)	42 (2)	64 (3)	3 (2)	−16 (3)	−6 (2)	3·1
C(4)	8185 (3)	902 (3)	4980 (3)	107 (5)	72 (3)	86 (3)	19 (3)	−12 (3)	−3 (3)	4·5
C(5)	9221 (4)	1132 (4)	4282 (3)	120 (5)	130 (5)	95 (4)	57 (4)	−6 (4)	8 (4)	5·9
C(6)	9867 (3)	2169 (5)	4289 (4)	68 (4)	177 (6)	104 (5)	13 (4)	−2 (4)	56 (4)	6·4
C(7)	9526 (4)	3000 (3)	5017 (4)	88 (5)	111 (5)	121 (5)	−20 (3)	−20 (4)	23 (4)	5·7
C(8)	8515 (3)	2754 (3)	5739 (3)	73 (4)	68 (3)	95 (3)	0 (3)	−24 (3)	4 (3)	4·2
C(9)	7838 (3)	1716 (3)	5717 (3)	72 (4)	58 (3)	73 (3)	10 (3)	−15 (3)	7 (3)	3·5
N(1′)	4538 (2)	2659 (2)	5924 (2)	68 (3)	51 (2)	100 (3)	−1 (2)	−26 (2)	14 (2)	3·9
C(2′)	3060 (3)	2427 (3)	5759 (3)	77 (4)	77 (3)	139 (4)	−4 (3)	−28 (3)	10 (3)	5·4
C(3′)	2396 (3)	1953 (3)	6722 (4)	90 (4)	100 (4)	138 (5)	−21 (3)	−8 (4)	14 (3)	5·9
C(4′)	3243 (4)	1078 (3)	7277 (3)	112 (5)	84 (4)	111 (4)	−30 (3)	−7 (4)	22 (3)	5·3
C(5′)	5603 (4)	242 (3)	7531 (3)	137 (5)	60 (3)	91 (3)	−5 (3)	−20 (3)	17 (3)	4·8
C(6′)	6847 (3)	638 (3)	7254 (3)	108 (4)	55 (3)	75 (3)	10 (3)	−18 (3)	−3 (2)	4·0
C(8′)	5252 (3)	1607 (2)	6162 (3)	82 (4)	43 (3)	83 (3)	−1 (2)	−25 (3)	1 (2)	3·6
C(9′)	4552 (3)	929 (3)	6990 (3)	108 (5)	56 (3)	84 (3)	−15 (3)	−20 (3)	−1 (3)	4·2
C(10′)	5058 (3)	3223 (3)	4993 (3)	105 (4)	76 (3)	118 (4)	6 (3)	−27 (3)	31 (3)	5·2
C(11′)	8142 (4)	210 (3)	7671 (3)	144 (5)	60 (3)	98 (4)	28 (3)	−24 (4)	−3 (3)	5·0
N(12′)	9175 (3)	−98 (3)	7979 (3)	160 (5)	105 (3)	127 (4)	61 (3)	−37 (3)	−1 (3)	6·7

Introduction. Intensity data were collected from a 0·35×0·15×0·10 mm crystal on a Philips PW 1100 diffractometer in a θ–2θ scan-mode using graphite-monochromated Cu $K\alpha$ radiation. 2651 independent reflexions were measured of which 1156 were considered as observed with $I > 3\sigma(I)$, $\sigma(I)$ being derived from counting statistics (Stout & Jensen, 1972).

The structure was solved by routine application of the phase function (Riche, 1973) and refined by full-matrix least-squares calculations (Busing, Martin & Levy, 1962). The function minimized was $\sum w(F_o - F_c)^2$ where w is the weight of an individual F derived from $\sigma(I)$.

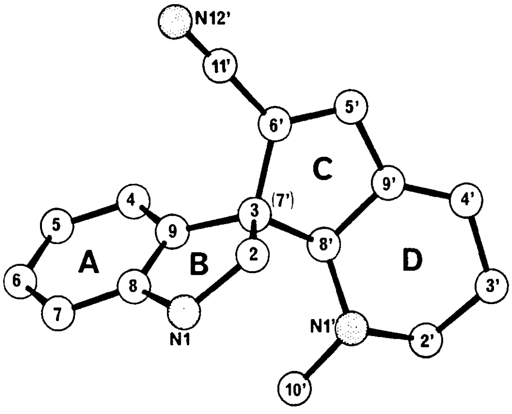


Fig. 1. A perspective view of the molecule.

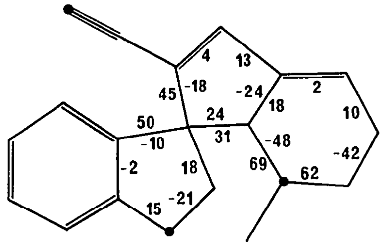


Fig. 2. Torsion angles (°).

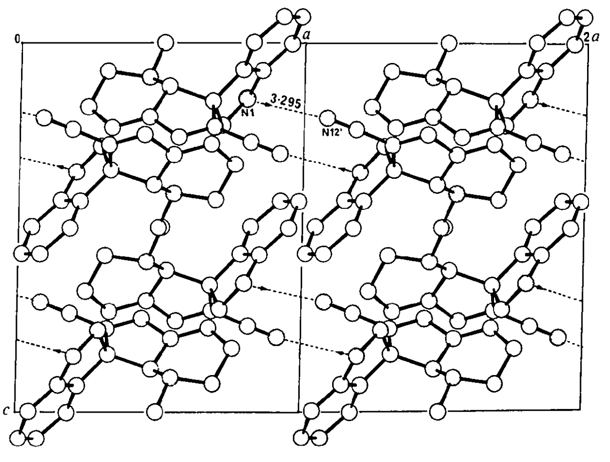


Fig. 3. Packing of the molecules down **b**.

The 17 hydrogen atoms were located in a difference map. They were assigned the equivalent isotropic thermal factor derived from the β of the bonded carbon atoms and included in the refinement in idealized positions (C–H = 1·00 Å, C–C–H = 109 or 120°). The final conventional R value was 0·062.*

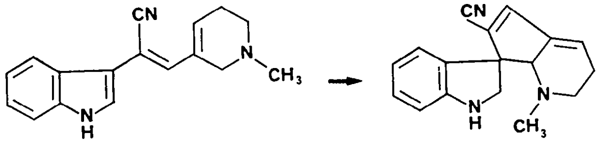
Scattering factors for carbon and nitrogen were those of Doyle & Turner (1968) and for hydrogen those of Stewart, Davidson & Simpson (1965).

The final atomic parameters are given in Tables 1 and 2.

Table 2. *Final coordinates* (×10³) *and B values for the hydrogen atoms* (*numbered according to the atom to which they are bonded*)

	x	y	z	B
H(N1)	876	384	691	4·6
H(2*A*)	629	319	741	3·9
H(2*B*)	768	258	788	3·9
H(4)	769	16	495	4·5
H(5)	951	54	376	5·9
H(6)	1060	232	376	6·4
H(7)	999	375	502	5·7
H(2'*A*)	259	315	556	5·4
H(2'*B*)	295	187	516	5·4
H(3'*A*)	223	259	723	5·9
H(3'*B*)	150	160	650	5·9
H(4')	292	57	786	5·3
H(5')	549	−41	803	4·8
H(8')	525	114	550	3·6
H(10'*A*)	470	402	497	5·2
H(10'*B*)	608	324	503	5·2
H(10'*C*)	474	280	434	5·2

Discussion. The irradiation of (I) resulted in the production of a photocyclization compound (II) which has been identified by the present X-ray analysis (Riche, Chiaroni, Doucerain, Besselièvre & Thal, 1975).



(I) (II)

The molecular structure of (II) and the atom numbering are shown in Fig. 1. It consists of two structural units: an indole and a pyrindine, spiro-joined at C(3). Bond lengths and valency angles involving non-hydrogen atoms are given in Table 3. Deviations from principal mean planes are listed in Table 4 and the endocyclic torsion angles are reported in Fig. 2.

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31716 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 3. *Bond lengths* (Å) *and angles* (°)

N(1)–C(2)	1·479 (4)	N(1′)—C(2′)	1·475 (4)
N(1)–C(8)	1·392 (5)	N(1′)—C(8′)	1·450 (4)
C(2)–C(3)	1·552 (4)	N(1′)—C(10′)	1·446 (5)
C(3)–C(9)	1·494 (4)	C(2′)—C(3′)	1·492 (6)
C(3)–C(6′)	1·507 (4)	C(3′)—C(4′)	1·486 (5)
C(3)–C(8′)	1·567 (4)	C(4′)—C(9′)	1·343 (6)
C(4)–C(5)	1·377 (5)	C(5′)—C(6′)	1·350 (5)
C(4)–C(9)	1·381 (5)	C(5′)—C(9′)	1·462 (5)
C(5)–C(6)	1·375 (7)	C(6′)—C(11′)	1·446 (5)
C(6)–C(7)	1·386 (7)	C(8′)—C(9′)	1·488 (5)
C(7)–C(8)	1·382 (5)	C(11′)–N(12′)	1·131 (5)
C(8)–C(9)	1·391 (5)		

C(2)–N(1)–C(8)	107·2 (3)	C(2′)–N(1′)—C(8′)	109·4 (3)
N(1)–C(2)–C(3)	105·4 (2)	C(2′)–N(1′)—C(10′)	109·1 (3)
C(2)–C(3)–C(9)	101·9 (2)	C(8′)–N(1′)—C(10′)	112·8 (3)
C(2)–C(3)–C(6′)	111·4 (3)	N(1′)–C(2′)—C(3′)	113·1 (3)
C(2)–C(3)–C(8′)	114·6 (2)	C(2′)–C(3′)—C(4′)	113·3 (3)
C(9)–C(3)–C(6′)	114·2 (3)	C(3′)–C(4′)—C(9′)	119·1 (3)
C(9)–C(3)–C(8′)	115·8 (3)	C(6′)–C(5′)—C(9′)	108·1 (3)
C(6′)–C(3)–C(8′)	99·6 (2)	C(3)—C(6′)—C(5′)	113·9 (3)
C(5)–C(4)–C(9)	118·8 (3)	C(3)—C(6′)—C(11′)	121·3 (3)
C(4)–C(5)–C(6)	120·8 (4)	C(5′)–C(6′)—C(11′)	124·4 (3)
C(5)–C(6)–C(7)	121·2 (4)	C(3)—C(8′)—N(1′)	117·7 (3)
C(6)–C(7)–C(8)	117·8 (4)	C(3)—C(8′)—C(9′)	104·6 (3)
N(1)–C(8)–C(7)	127·4 (3)	N(1′)–C(8′)—C(9′)	112·3 (3)
N(1)–C(8)–C(9)	111·4 (3)	C(4′)–C(9′)—C(5′)	127·4 (3)
C(7)–C(8)–C(9)	121·0 (3)	C(4′)–C(9′)—C(8′)	124·6 (3)
C(3)–C(9)–C(4)	129·8 (3)	C(5′)–C(9′)—C(8′)	107·3 (3)
C(3)–C(9)–C(8)	109·9 (3)	C(6′)–C(11′)–N(12′)	177·8 (4)
C(4)–C(9)–C(8)	120·2 (3)		

The two five-membered rings *B* and *C* have a conformation intermediate between a flattened envelope and a flattened half-chair as indicated by the values of the pseudorotation phase angle Δ and the maximum torsion angle φ_m (Altona, Geise & Romers, 1968): $\Delta=20$, $\varphi_m=21°$ for ring *B* [near $C_s(2)$ envelope] and $\Delta=22$, $\varphi_m=26°$ for ring *C* [near $C_s(8)$ envelope]. Ring *D* has an almost ideal half-chair conformation as calculated by Bucourt & Hainaut (1965) for an unsubstituted cyclohexene. The methyl group C(10′) is in an equatorial position. The four atoms C(3′), C(4′), C(9′) and C(8′) are in a quite planar configuration while the atoms C(9′), C(5′), C(6′) and C(7′) are slightly displaced from their least-squares mean plane, the atoms C(11′) and N(12′) being widely out of this plane. The angle between these two double-bond planes is 19°.

The packing of the molecules is illustrated in Fig. 3. The nitrogen of the cyano group participates as acceptor in a weak intermolecular hydrogen bond N(1)–H···N(12′) (N···N = 3·295 (4), H···N = 2·37 Å; N–H···N = 153°) linking molecules in zigzag chains along **b**.

Table 4. *Principal least-squares planes and atomic deviations* (*in* Å) *from the planes*

Atoms marked with an asterisk are included in the plane calculation. The general equation for the plane is $lX+mY+nZ+P=0$ where X, Y and Z are the coordinates in Å with respect to the orthogonal axes a, b and c^* and P is the origin to the plane distance in Å.

Plane *A*	$0{\cdot}6706X-0{\cdot}3660Y+0{\cdot}6453Z-8{\cdot}9130=0$
Plane *C′*	$-0{\cdot}0326X+0{\cdot}5903Y+0{\cdot}8065Z-7{\cdot}6021=0$
Plane *D′*	$0{\cdot}2740X+0{\cdot}6696Y+0{\cdot}6903Z-7{\cdot}9679=0$

Plane *A* (mean e.s.d. 0·004 Å except for the H atoms)

C(4)*	−0·008	N(1)	−0·039	C(6′)	1·037
C(5)*	0·015	C(2)	0·276	C(8′)	−1·289
C(6)*	−0·005	C(3)	−0·004	C(10′)	−3·042
C(7)*	−0·010	H(N1)	0·63		
C(8)*	0·010	H(2*A*)	−0·31		
C(9)*	−0·002	H(2*B*)	1·23		

Plane *C′* (mean e.s.d. 0·003 Å)

C(3)*	0·010	C(8′)	−0·402	C(2)	1·413
C(6′)*	−0·021	C(11′)	0·063	N(1′)	0·112
C(5′)*	0·024	N(12′)	0·127	C(4′)	0·423
C(9′)*	−0·012	H(5′)	0·073		

Plane *D′* (mean e.s.d. 0·003 Å)

C(8′)*	0·003	N(1′)	0·439	C(3)	0·817
C(9′)*	−0·007	C(2′)	−0·281	C(6′)	0·602
C(4′)*	0·008	C(10′)	0·223	C(5′)	0·196
C(3′)*	−0·004	H(4′)	0·03	C(2)	2·327
		H(8′)	−0·94		

We wish to thank Dr Claude Thal for suggesting the problem and for interesting discussions.

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