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6-Cyano-7:2′-(1′-aminophenyl)isoquinoline

BY ANGÈLE CHIARONI, HERVÉ DOUCERAIN AND CLAUDE RICHE

Institut de Chimie des Substances Naturelles, CNRS, 91190 Gif/Yvette, France

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Abstract. $C_{16}H_{11}N_3$, $M=245{\cdot}25$; monoclinic, $P2_1/c$; $a=8{\cdot}066$ (4), $b=6{\cdot}563$ (3), $c=23{\cdot}849$ (7) Å, $\beta=93{\cdot}4$ (1)°, $Z=4$, $d_{calc}=1{\cdot}29$ g cm^{-3}. The structure has been refined by full-matrix least-squares calculations to a final R value of 0·068 with 1221 observed intensities.

Introduction. Intensity data were collected from a 0·5 × 0·3 × 0·1 mm crystal on a Philips PW1100 diffractometer. 1959 independent reflexions were measured of which 1221 were considered as observed with $I>3\sigma(I)$, $\sigma(I)$ being derived from counting statistics (Stout & Jensen, 1972). The structure was solved by use of the multiple solution weighted tangent formula procedure (Germain, Main & Woolfson, 1971) 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 for an individual F derived from $\sigma(I)$.

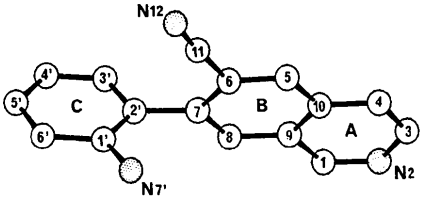


Fig. 1. A perspective view of the molecule.

All the hydrogen atoms were located in a difference map. They were assigned the equivalent isotropic thermal factor of the bonded carbon. Only coordinates of the amino group hydrogens were refined. The other hydrogen atoms were included in the refinement at theoretical positions (C–H = 1·0 Å). The final R was 0·068.* Scattering factors for carbon and nitrogen

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31717 (10 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

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(1)	559	−378	478	5·1
H(3)	718	−195	628	5·9
H(4)	843	101	595	5·2
H(5)	902	329	509	4·6
H(8)	626	−167	390	4·5
H(3′)	893	−116	314	6·1
H(4′)	898	−57	217	7·7
H(5′)	768	225	175	7·6
H(6′)	609	453	228	6·7
H(N*A*′)	491	510	316	6·7
H(N*B*′)	529	386	381	6·7

Table 1. *Final coordinates and thermal parameters* (× 10⁴) *and their e.s.d.'s for the non-hydrogen atoms*

B is the equivalent isotropic thermal factor. The expression used for temperature factors is:

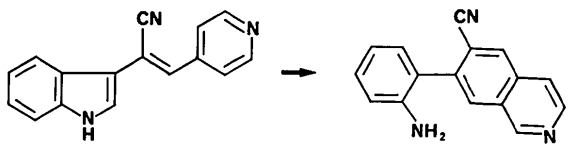
$$\exp\left[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)\right].$$

	x	*y*	*z*	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	*B*
C(1)	6210 (4)	−2695 (5)	4996 (2)	217 (7)	186 (9)	29 (1)	−29 (6)	7 (2)	4 (2)	5·1
N(2)	6278 (4)	−3059 (4)	5531 (1)	267 (6)	246 (8)	25 (1)	−17 (6)	4 (2)	15 (2)	5·6
C(3)	7103 (5)	−1674 (6)	5870 (1)	256 (8)	337 (12)	23 (1)	2 (8)	7 (2)	8 (3)	5·9
C(4)	7829 (4)	65 (5)	5677 (1)	218 (7)	266 (10)	24 (1)	−29 (7)	3 (2)	2 (2)	5·2
C(5)	8421 (4)	2221 (4)	4860 (1)	193 (6)	201 (8)	23 (1)	−42 (6)	1 (2)	−3 (2)	4·6
C(6)	8290 (3)	2491 (4)	4293 (1)	152 (6)	174 (8)	22 (1)	−25 (6)	5 (2)	−2 (2)	4·0
C(7)	7504 (3)	1065 (4)	3919 (1)	159 (6)	179 (8)	21 (1)	−6 (6)	5 (2)	−4 (2)	4·0
C(8)	6828 (4)	−648 (4)	4155 (1)	195 (6)	174 (8)	23 (1)	−20 (6)	4 (2)	−9 (2)	4·5
C(9)	6928 (3)	−966 (4)	4738 (1)	169 (6)	169 (8)	22 (1)	−5 (6)	5 (2)	0 (2)	4·1
C(10)	7714 (3)	462 (5)	5101 (1)	153 (6)	211 (8)	21 (1)	11 (6)	2 (2)	−2 (2)	4·1
C(11)	9090 (4)	4255 (5)	4068 (1)	220 (7)	242 (10)	21 (1)	−40 (7)	3 (2)	−8 (2)	4·9
N(12)	9792 (4)	5629 (4)	3911 (1)	308 (7)	279 (9)	27 (1)	−96 (7)	0 (2)	1 (2)	6·4
C(1′)	6617 (4)	3043 (5)	3056 (2)	216 (7)	239 (10)	25 (1)	−33 (7)	−1 (2)	7 (3)	5·1
C(2′)	7441 (4)	1393 (5)	3303 (1)	192 (7)	225 (9)	21 (1)	−29 (6)	−1 (2)	5 (2)	4·6
C(3′)	8325 (5)	52 (5)	2970 (1)	281 (8)	368 (12)	21 (1)	−56 (8)	16 (2)	−15 (3)	6·1
C(4′)	8369 (5)	394 (8)	2406 (2)	329 (10)	482 (16)	28 (1)	−46 (10)	13 (3)	−26 (4)	7·7
C(5′)	7588 (6)	2030 (8)	2162 (2)	330 (11)	509 (17)	24 (1)	−125 (11)	15 (3)	5 (4)	7·6
C(6′)	6683 (5)	3366 (6)	2471 (2)	273 (9)	367 (13)	29 (1)	−76 (9)	−13 (2)	37 (3)	6·7
N(7′)	5762 (4)	4377 (5)	3374 (2)	275 (7)	320 (10)	35 (1)	49 (7)	0 (2)	27 (3)	6·9

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.

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



(I) (II)

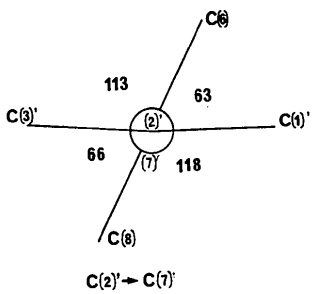


Fig. 2. Newman projection along the C(2′)–C(7) bond, angles in (°).

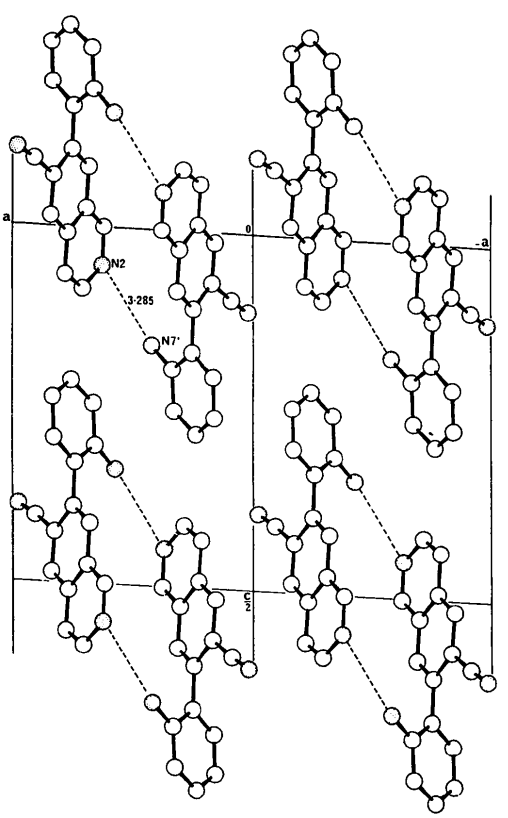


Fig. 3. Packing of the molecules down **b**.

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

The mean e.s.d. on angles is 0·3° [2° for those involving atom N(7′)].

C(1)–N(2)	1·296 (5)	C(8)—C(9)	1·404 (5)
C(1)–C(9)	1·429 (4)	C(9)—C(10)	1·402 (4)
N(2)–C(3)	1·364 (5)	C(11)–N(12)	1·139 (5)
C(3)–C(4)	1·374 (5)	C(1′)–C(2′)	1·384 (5)
C(4)–C(10)	1·395 (5)	C(1′)–C(6′)	1·414 (6)
C(5)–C(6)	1·361 (5)	C(1′)–N(7′)	1·371 (5)
C(5)–C(10)	1·423 (4)	C(2′)–C(3′)	1·406 (5)
C(6)–C(7)	1·417 (4)	C(3′)–C(4′)	1·368 (6)
C(6)–C(11)	1·445 (4)	C(4′)–C(5′)	1·358 (7)
C(7)–C(8)	1·383 (4)	C(5′)–C(6′)	1·382 (6)
C(7)–C(2′)	1·484 (4)	N(7′)–H(N*A*′)	0·95 (3)
		N(7′)–H(N*B*′)	1·19 (3)

N(2)–C(1)–C(9)	125·1	C(4)——C(10)–C(5)	122·9
C(1)–N(2)–C(3)	116·8	C(4)——C(10)–C(9)	119·0
N(2)–C(3)–C(4)	123·9	C(5)——C(10)–C(9)	118·0
C(3)–C(4)–C(10)	118·6	C(6)——C(11)–N(12)	176·2
C(6)–C(5)–C(10)	119·8	C(2′)——C(1′)–C(6′)	119·5
C(5)–C(6)–C(7)	123·0	C(2′)——C(1′)–N(7′)	120·6
C(5)–C(6)–C(11)	117·7	C(6′)——C(1′)–N(7′)	119·9
C(7)–C(6)–C(11)	119·2	C(7)——C(2′)–C(1′)	121·5
C(6)–C(7)–C(8)	117·0	C(7)——C(2′)–C(3′)	118·6
C(6)–C(7)–C(2′)	121·1	C(1′)——C(2′)–C(3′)	119·8
C(8)–C(7)–C(2′)	121·9	C(2′)——C(3′)–C(4′)	119·7
C(7)–C(8)–C(9)	121·4	C(3′)——C(4′)–C(5′)	120·9
C(1)–C(9)–C(8)	122·9	C(4′)——C(5′)–C(6′)	121·3
C(1)–C(9)–C(10)	116·4	C(1′)——C(6′)–C(5′)	118·9
C(8)–C(9)–C(10)	120·7	C(1′)——N(7′)–H(N*A*′)	113
		C(1′)——N(7′)–H(N*B*′)	120
		H(N*A*′)–N(7′)–H(N*B*′)	111

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

Atoms included in the calculation of the plane are marked with an asterisk. 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* $0{\cdot}8641X-0{\cdot}4965Y-0{\cdot}0826Z-3{\cdot}6241=0$
Plane *B* $0{\cdot}8729X-0{\cdot}4827Y-0{\cdot}0713Z-3{\cdot}8003=0$
Plane (*A*+*B*) $0{\cdot}8682X-0{\cdot}4902Y-0{\cdot}0768Z-3{\cdot}7117=0$
Plane *C* $-0{\cdot}8129X-0{\cdot}5581Y-0{\cdot}1662Z+6{\cdot}3171=0$

	Plane *A*	Plane *B*	Plane (*A*+*B*)
C(1)	−0·004 (3)*	−0·032 (3)	−0·015 (3)*
N(2)	−0·007 (3)*	−0·024 (3)	−0·014 (3)*
C(3)	0·008 (4)*	0·018 (4)	0·015 (4)*
C(4)	0·009 (3)*	0·035 (3)	0·023 (3)*
C(5)	−0·022 (3)	0·006 (3)*	−0·008 (3)*
C(6)	−0·021 (3)	−0·006 (3)*	−0·014 (3)*
C(7)	0·015 (3)	0·002 (3)*	0·008 (3)*
C(8)	0·027 (3)	0·000 (3)*	0·014 (3)*
C(9)	0·015 (3)*	0·001 (3)*	0·009 (3)*
C(10)	−0·018 (3)*	−0·004 (3)*	−0·010 (3)*
C(11)	0·034 (3)	0·065 (3)	0·047 (3)
N(12)	0·125 (3)	0·169 (3)	0·145 (3)
C(2′)	0·059 (3)	0·033 (3)	0·046 (3)
C(1′)	−0·974 (3)	−0·997 (3)	−0·986 (3)

Plane *C*

C(1′)	0·002 (3)*	C(6′)	0·005 (4)
C(2′)	0·003 (3)*	N(7′)	−0·016 (3)
C(3′)	0·001 (4)*	H(N*A*′)	0·33 (3)
C(4′)	0·007 (4)*	H(N*B*′)	0·36 (3)
C(5′)	−0·012 (5)*		

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′-pyrindine)]

BY ANGÈLE CHIARONI, HERVÉ DOUCERAIN AND CLAUDE RICHE

Institut de Chimie des Substances Naturelles, CNRS, 91190 *Gif/Yvette, France*

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Abstract. $C_{17}H_{17}N_3$, $M = 265{\cdot}35$; monoclinic $P2_1/c$; $a = 9{\cdot}736$ (7), $b = 11{\cdot}791$ (12), $c = 12{\cdot}566$ (10) Å, $\beta = 91{\cdot}15$ (8)°, $V = 1442{\cdot}3$ Å^3; $Z = 4$, $d_{calc} = 1{\cdot}22$ 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* ($\times 10^4$) *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