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Structure of 4-Azadibenzofuran-3-carbonitrile

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Abstract. Pyridino[3,2-*b*][1]benzofuran-2-carbonitrile, $C_{12}H_6N_2O$, $M_r = 194.2$, triclinic, $P\bar{1}$, $a = 10.888$ (1), $b = 7.381$ (1), $c = 6.541$ (1) Å, $\alpha = 114.95$ (1), $\beta = 79.82$ (1), $\gamma = 105.24°$, $U = 458.9$ (2) Å^3, $Z = 2$, $D_x = 1.40$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.54178 Å, $\mu = 0.767$ mm^{-1}, $F(000) = 200$, $T = 293$ K, final $R = 0.049$ for 1324 reflections. The dibenzofuran ring system lies in a plane which also includes the cyano group. This is indicative of extensive electron delocalization.

Experimental. A clear $0.35 \times 0.15 \times 0.45$ mm crystal, obtained by recrystallization from $C_2H_5OC_2H_5$, was used for data collection. Rigaku AFC5 four-circle diffractometer used with θ–2θ scan method, ω scan width $(1.3 + 0.41\tan\theta)°$ and scan speed 16° min^{-1}. Lattice parameters obtained from least-squares analysis of 20 reflections with 2θ values ranging from 32 to 65°. Of 1332 reflections scanned within the index range h −12 to 12, k −8 to 8, l 0 to 7 and up to $\sin\theta/\lambda \le 0.56$ Å^{-1}, there were 1324 unique reflections with $F > 3\sigma(F)$ which were counted as observed. Three standard reflections measured every 150 reflections showed no significant variation in intensity. Intensities corrected for Lorentz and polarization factors, but not for absorption. Structure solved using program package *SAPI85* (Yao, Zheng, Qian, Han, Gu & Fan, 1985) version of *MULTAN80* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). The refinement was carried out by the full-matrix least-squares method with anisotropic temperature factors for non-H atoms. The function minimized was $\sum w[(|F_o|)^2 - (|F_c|)^2]^2$ with $w = 1/[\sigma^2(F_o) + 0.02 \times (F_o)^2]$, $\sigma(F_o)$ determined from counting statistics.

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All H atoms located from the difference map and refined; the initial thermal parameters were set at an equivalent isotropic thermal parameter for each bonded atom. Final discrepancy indices $R = 0.049$, $wR = 0.050$, $S = 1.726$ for 1324 reflections. Maximum $\Delta/\sigma = 0.28$ in final least-squares cycle. Final maximum and minimum difference Fourier residuals 0.16 and −0.39 e Å^{-3}. All computations performed on a Panafacom computer with *RCRYSTAN* (Rigaku Corporation, 1985) X-ray analysis program system. The atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV).

Final atomic parameters are listed in Table 1.* The bond lengths and angles are listed in Table 2.

Table 1. *Fractional atomic coordinates and isotropic thermal parameters* (Å^2)

$$B_{eq} = (1/3)\sum_i\sum_j B_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
N(1)	1.1427 (1)	0.7524 (2)	−0.1688 (2)	4.48 (4)
C(2)	1.0439 (1)	0.7538 (2)	−0.0161 (2)	3.87 (5)
C(3)	1.0561 (1)	0.7826 (2)	0.2056 (2)	4.21 (5)
C(4)	1.1719 (1)	0.8115 (2)	0.2835 (3)	5.07 (6)
C(5)	1.2747 (1)	0.8116 (2)	0.1276 (3)	5.18 (6)
C(6)	1.2564 (1)	0.7832 (2)	−0.0917 (2)	4.69 (6)
C(7)	1.3648 (1)	0.7843 (3)	−0.2525 (4)	5.91 (7)
N(8)	1.4521 (1)	0.7840 (3)	−0.3782 (4)	8.35 (9)
O(9)	0.9406 (1)	0.7788 (1)	0.3279 (2)	5.02 (4)
C(10)	0.9093 (1)	0.7271 (2)	−0.0331 (2)	4.12 (5)
C(11)	0.8328 (1)	0.6899 (3)	−0.2024 (3)	5.28 (6)
C(12)	0.7030 (1)	0.6753 (3)	−0.1476 (4)	6.07 (7)
C(13)	0.6491 (1)	0.6966 (3)	0.0675 (4)	5.95 (7)
C(14)	0.7230 (1)	0.7325 (3)	0.2384 (3)	5.30 (6)
C(15)	0.8517 (1)	0.7447 (2)	0.1799 (3)	4.34 (5)

Table 2. *Bond lengths* (Å) *and angles* (°)

N(1)—C(2)	1·332 (2)	O(9)—C(15)	1·391 (3)
C(2)—C(3)	1·400 (3)	C(10)—C(11)	1·395 (3)
C(2)—C(10)	1·444 (3)	C(11)—C(12)	1·383 (3)
C(3)—C(4)	1·374 (3)	C(12)—C(13)	1·386 (4)
C(3)—O(9)	1·367 (2)	C(13)—C(14)	1·387 (4)
C(4)—C(5)	1·376 (3)	C(14)—C(15)	1·375 (3)
C(5)—C(6)	1·403 (3)	C(15)—C(10)	1·392 (3)
C(6)—N(1)	1·347 (3)		
C(6)—C(7)	1·437 (3)		
C(7)—N(8)	1·141 (3)		

N(1)—C(2)—C(3)	123·1 (1)	O(9)—C(15)—C(14)	124·0 (1)
N(1)—C(2)—C(10)	130·8 (1)	O(9)—C(15)—C(10)	111·6 (1)
C(2)—C(3)—C(4)	122·5 (1)	C(10)—C(2)—C(3)	106·0 (1)
C(2)—C(3)—O(9)	111·4 (1)	C(10)—C(11)—C(12)	117·8 (2)
C(3)—C(4)—C(5)	114·8 (2)	C(11)—C(12)—C(13)	121·8 (2)
C(4)—C(5)—C(6)	119·9 (2)	C(12)—C(13)—C(14)	121·5 (2)
C(5)—C(6)—N(1)	125·1 (1)	C(13)—C(14)—C(15)	115·7 (2)
C(5)—C(6)—C(7)	119·3 (2)	C(14)—C(15)—C(10)	124·2 (2)
C(6)—C(7)—N(8)	178·7 (3)	C(15)—C(10)—C(11)	118·8 (1)
C(6)—N(1)—C(2)	114·3 (1)		
C(7)—C(6)—N(1)	115·5 (2)		
O(9)—C(3)—C(4)	126·0 (1)		

Fig. 1 shows a thermal-ellipsoid plot of the molecule with atomic labeling.

Related literature. The title compound was obtained by flash vacuum pyrolysis of 2-cyano-6-phenylpyridine *N*-oxide (Itoh, Ohsawa, Itoh & Igeta, 1990).
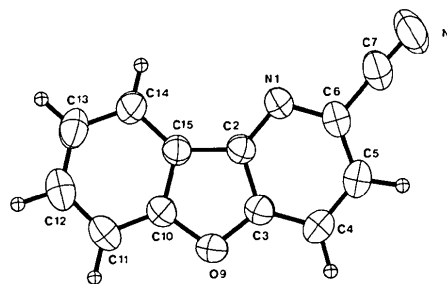

Fig. 1. Thermal-ellipsoid plot (Johnson, 1965). Ellipsoids are drawn at the 50% probability level while isotropic hydrogen thermal parameters are represented by spheres of arbitrary size.

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Structure of 3-(1-Aziridinyl)-*N*-(*p*-chlorophenyl)succinimide*

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Abstract. $C_{12}H_{11}ClN_2O_2$, $M_r = 250 \cdot 7$, monoclinic, $P2_1/a$, $a = 8\cdot328$ (4), $b = 11\cdot017$ (5), $c = 12\cdot763$ (2) Å, $\beta = 93\cdot99$ (4)°, $V = 1168$ (1) Å^3, $Z = 4$, $D_x = 1\cdot43$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0\cdot7107$ Å, $\mu = 0\cdot314$ mm^{-1}, $F(000) = 520$, $T = 293$ K, $R = 0\cdot045$ for 1267 observed reflections. The X-ray analysis establishes unequivocally the molecular structure of the title compound. The aziridinyl ring is planar. The succinimide ring is a β-envelope with C(2) as the flap