

Table 2. Bond distances (Å) and angles (°)

S—O3	1.434 (2)	C10—C15	1.363 (5)
S—O4	1.439 (3)	C11—C12	1.392 (4)
S—C4	1.765 (3)	C12—C13	1.377 (4)
S—C16	1.754 (3)	C13—C14	1.358 (4)
O1—C7	1.364 (3)	C14—C15	1.408 (6)
O1—C10	1.412 (3)	C16—C17	1.392 (4)
O2—C19	1.379 (4)	C16—C21	1.388 (4)
O2—C22	1.412 (4)	C17—C18	1.382 (4)
N1—C13	1.406 (5)	C18—C19	1.370 (4)
N2—C25	1.391 (4)	C19—C20	1.376 (4)
C4—C5	1.390 (4)	C20—C21	1.382 (4)
C4—C9	1.391 (4)	C22—C23	1.373 (3)
C5—C6	1.373 (5)	C22—C27	1.371 (4)
C6—C7	1.391 (5)	C23—C24	1.391 (4)
C7—C8	1.383 (4)	C24—C25	1.396 (4)
C8—C9	1.384 (3)	C25—C26	1.396 (3)
C10—C11	1.374 (4)	C26—C27	1.373 (4)
C4—S—C16	107.6 (1)	C12—C13—C14	120.2 (3)
O4—S—C16	108.3 (1)	N1—C13—C14	119.8 (3)
O4—S—C4	106.9 (1)	C13—C14—C15	120.3 (3)
O3—S—C16	107.8 (1)	C10—C15—C14	119.1 (2)
O3—S—C4	106.9 (1)	S—C16—C21	120.8 (2)
O3—S—O4	118.9 (1)	S—C16—C17	119.2 (2)
C7—O1—C10	119.5 (2)	C17—C16—C21	120.0 (2)
C19—O2—C22	119.0 (2)	C16—C17—C18	119.8 (2)
S—C4—C9	120.4 (2)	C17—C18—C19	119.5 (2)
S—C4—C5	119.4 (2)	O2—C19—C18	123.5 (2)
C5—C4—C9	120.1 (2)	C18—C19—C20	121.3 (2)
C4—C5—C6	119.7 (2)	O2—C19—C20	115.2 (2)
C5—C6—C7	120.1 (3)	C19—C20—C21	119.7 (2)
O1—C7—C6	114.8 (2)	C16—C21—C20	119.6 (2)
C6—C7—C8	120.7 (2)	O2—C22—C27	118.3 (2)
O1—C7—C8	124.5 (2)	O2—C22—C23	120.7 (2)
C7—C8—C9	119.2 (2)	C23—C22—C27	120.8 (2)
C4—C9—C8	120.2 (2)	C22—C23—C24	119.3 (2)
O1—C10—C15	118.3 (2)	C23—C24—C25	120.9 (2)
O1—C10—C11	120.6 (2)	N2—C25—C24	121.7 (2)
C11—C10—C15	120.9 (3)	C24—C25—C26	117.9 (2)
C10—C11—C12	119.5 (2)	N2—C25—C26	120.4 (2)
C11—C12—C13	119.9 (2)	C25—C26—C27	120.9 (2)
N1—C13—C12	119.9 (2)	C22—C27—C26	120.2 (2)

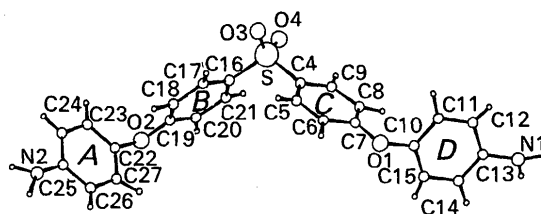


Fig. 1. Projection of the molecule.

Atomic parameters for non-H atoms are given in Table 1;* Table 2 contains bond distances and angles while the arbitrary labelling of atoms is shown in Fig. 1.

Related literature. This structure is one of a series of oligomers related to polymers which are of interest because of their technological properties.

* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates with their isotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53028 (22 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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= 0.057. Atomic scattering factors from *SHELX76*. All calculations performed on an IBM PS2/80 personal computer with the *CRYSRULER* package (Rizzoli, Sangermano, Calestani & Andreotti, 1987).

Acta Cryst. (1990). **C46**, 2260–2262

Structure of 6-(2-Hydroxyphenyl)pyridine-2-carbonitrile

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(Received 29 March 1990; accepted 1 May 1990)

Abstract. $C_{12}H_8N_2O$, $M_r = 196.2$, monoclinic, $C2/c$, $a = 11.768$ (2), $b = 8.057$ (1), $c = 21.363$ (4) Å, $\beta = 106.83$ (1)°, $U = 1938.7$ (4) Å³, $Z = 8$, $D_x = 1.344$ Mg m⁻³, $\lambda(\text{Cu } K\alpha) = 1.54178$ Å, $\mu = 0.727$ mm⁻¹, $F(000) = 816$, $T = 293$ K, final $R = 0.060$ for 1688 reflections. The dihedral angle between the pyridine and phenyl rings is 1.4 (1)°. An

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intramolecular hydrogen bond exists between the OH and the pyridyl N atom with a distance of 2.586 (2) Å.

Experimental. A yellow 0.25 × 0.10 × 0.35 mm crystal, obtained by recrystallization from CHCl₃, was used for data collection. Rigaku AFC5 four-circle diffractometer used with θ -2 θ scan method, ω scan width (1.3 + 0.41 tan θ)° and scan speed 16° min⁻¹. Lattice parameters obtained from least-squares analysis of 20 reflections with 2 θ values ranging from 55 to 60°. Of 1716 reflections scanned within the index range h - 14 to 14, k 0 to 9, l 0 to 25 and up to $\sin\theta/\lambda \leq 0.56$ Å⁻¹, there were 1688 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. All H atoms located from a difference map and refined. The initial thermal parameters were set at an equivalent isotropic thermal parameter for each bonded atom. Final discrepancy indices $R = 0.060$, $wR = 0.064$, $S = 2.171$ for 1688 reflections. Maximum $\Delta/\sigma = 0.13$ in final least-squares cycle. Final maximum and minimum difference Fourier residuals 0.12 and -0.19 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. Fig. 1 shows a thermal-ellipsoid plot of the molecule with atomic labeling.

Related literature. The title compound is one of the products obtained from flash vacuum pyrolysis of 2-cyano-6-phenylpyridine *N*-oxide (Itoh, Ohsawa, Itoh & Igeta, 1990).

* Lists of structure amplitudes, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53055 (6 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates and isotropic thermal parameters (Å²)*

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

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq}
N(1)	0.3499 (1)	0.1966 (1)	-0.0658 (1)	3.18 (3)
C(2)	0.2808 (1)	0.2036 (1)	-0.1278 (1)	3.54 (3)
C(3)	0.1798 (1)	0.1093 (2)	-0.1525 (1)	4.11 (4)
C(4)	0.1489 (1)	0.0018 (2)	-0.1097 (1)	4.44 (4)
C(5)	0.2179 (1)	-0.0088 (1)	-0.0459 (1)	3.92 (4)
C(6)	0.3206 (1)	0.0906 (1)	-0.0244 (1)	3.03 (3)
C(7)	0.3190 (1)	0.3188 (2)	-0.1696 (1)	4.61 (4)
N(8)	0.3481 (1)	0.4081 (2)	-0.2035 (1)	6.87 (6)
C(9)	0.3993 (1)	0.0846 (1)	0.0433 (1)	3.09 (3)
C(10)	0.5005 (1)	0.1870 (1)	0.0649 (1)	3.28 (3)
C(11)	0.5719 (1)	0.1781 (2)	0.1295 (1)	3.98 (4)
C(12)	0.5457 (1)	0.0694 (2)	0.1727 (1)	4.41 (4)
C(13)	0.4473 (1)	-0.0330 (2)	0.1528 (1)	4.56 (4)
C(14)	0.3758 (1)	-0.0245 (1)	0.0892 (1)	3.90 (4)
O(15)	0.5330 (1)	0.2976 (1)	0.0257 (1)	4.26 (3)

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

N(1)—C(2)	1.341 (2)	C(9)—C(10)	1.412 (2)
N(1)—C(6)	1.343 (2)	C(10)—O(15)	1.352 (2)
C(2)—C(3)	1.381 (2)	C(10)—C(11)	1.395 (2)
C(2)—C(7)	1.446 (3)	C(11)—C(12)	1.371 (3)
C(3)—C(4)	1.382 (3)	C(12)—C(13)	1.385 (3)
C(4)—C(5)	1.373 (2)	C(13)—C(14)	1.378 (2)
C(5)—C(6)	1.412 (2)	C(14)—C(9)	1.403 (2)
C(6)—C(9)	1.475 (2)	C(7)—N(8)	1.141 (3)
N(1)—C(2)—C(3)	124.2 (1)	C(9)—C(10)—C(11)	120.2 (1)
N(1)—C(2)—C(7)	115.4 (2)	C(9)—C(10)—O(15)	123.0 (1)
N(1)—C(6)—C(9)	117.2 (1)	C(10)—C(11)—C(12)	120.6 (1)
C(2)—C(3)—C(4)	116.9 (1)	C(11)—C(12)—C(13)	120.3 (1)
C(2)—C(7)—C(8)	178.7 (2)	C(11)—C(10)—O(15)	116.7 (1)
C(3)—C(4)—C(5)	120.2 (1)	C(12)—C(13)—C(14)	119.3 (1)
C(3)—C(2)—C(7)	120.2 (1)	C(13)—C(14)—C(9)	122.2 (1)
C(4)—C(5)—C(6)	119.4 (1)	C(14)—C(9)—C(10)	117.1 (1)
C(5)—C(6)—N(1)	120.3 (1)		
C(5)—C(6)—C(9)	122.3 (1)		
C(6)—N(1)—C(2)	118.7 (1)		
C(6)—C(9)—C(14)	120.7 (1)		
C(6)—C(9)—C(10)	122.1 (1)		

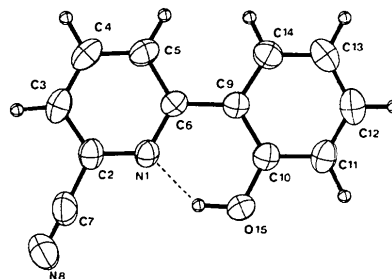


Fig. 1. Thermal-ellipsoid plot (Johnson, 1965). Ellipsoids are drawn at the 50% probability level while isotropic hydrogen thermal parameters are represented by spheres of arbitrary size. The hydrogen bond is represented by a dashed line.

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Acta Cryst. (1990). **C46**, 2262–2263

Structure of 4-Azadibenzofuran-3-carbonitrile

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(Received 29 March 1990; accepted 1 May 1990)

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), $\gamma = 105.24^\circ$, $U = 458.9$ (2) Å³, $Z = 2$, $D_x = 1.40$ Mg m⁻³, $\lambda(\text{Cu } K\alpha) = 1.54178$ 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 $(1.3 + 0.41 \tan \theta)^\circ$ and scan speed $16^\circ \text{ min}^{-1}$. 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 $\sin \theta / \lambda \leq 0.56$ 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.

* Lists of structure amplitudes, anisotropic thermal parameters, H-atom parameters and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53056 (5 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates and isotropic thermal parameters (Å²)*

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

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{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 (3)	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)