

Table 1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic vibration parameters ($\text{\AA}^2 \times 10^3$) for non-H atoms

$$U_{\text{eq}} = \frac{1}{3}(U_{11} + U_{22} + U_{33}).$$

	x	y	z	U_{eq}
F(1)	2772 (6)	-9 (4)	2924 (3)	92 (4)
N(1)	4529 (11)	841 (7)	960 (5)	85 (8)
N(2)	10625 (9)	2778 (5)	2917 (5)	63 (5)
O(1)	3083 (12)	-22 (7)	928 (5)	137 (9)
O(2)	5089 (11)	1509 (7)	256 (4)	143 (9)
O(3)	11465 (7)	3050 (5)	2090 (4)	80 (5)
O(4)	11403 (8)	3118 (5)	3767 (4)	92 (5)
C(1)	4716 (9)	596 (6)	2914 (6)	59 (5)
C(2)	5598 (9)	1072 (6)	1977 (5)	59 (5)
C(3)	7574 (10)	1784 (5)	1972 (4)	52 (5)
C(4)	8561 (8)	1974 (6)	2912 (5)	50 (5)
C(5)	7708 (11)	1510 (6)	3837 (5)	61 (6)
C(6)	5783 (11)	832 (6)	3833 (5)	61 (7)

$3\sigma(I)$ used in refinement. Phase solution by use of *MULTAN78* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). *SHELX76* (Sheldrick, 1976) used for all other calculations including ΔF map (for H positions), least-squares refinement (based on F) of positions and U_{ij} of non-H atoms, of isotropic U of H atoms riding on parent C atoms with C—H = 1.08 Å. Interlayer scale factors refined at an intermediate stage, final $\Delta/\sigma < 0.02$, variations in final ΔF map 0.19 to -0.18 e \AA^{-3} . Final $R = 0.057$, $wR = 0.065$, $w = 4.231/[\sigma^2(F) + 0.00012F^2]$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). Atomic parameters are listed in Table 1,* bond distances and angles in Table 2, and the molecule with atomic labelling is shown in Fig. 1.

* Lists of torsion angles, structure factors, H-atom coordinates, anisotropic vibrational factors and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53331 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 2,6-Dimethylbenzotrile

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Abstract. $\text{C}_9\text{H}_9\text{N}$, $M_r = 131.1$, monoclinic, $a = 14.779$ (16), $b = 7.654$ (8), $c = 16.488$ (15) Å, $\beta = 124.8$ (1)°, $V = 1531.5$ Å³, $F(000) = 560$, $D_x = 1.14 \text{ g cm}^{-3}$, $Z = 8$, MoK α radiation ($\lambda = 0.7107$ Å), $\mu(\text{Mo K}\alpha) = 0.73 \text{ cm}^{-1}$, $T = 293 \text{ K}$. Space group $A2/a$ (non-standard setting of $C2/c$ with $a \rightarrow c$ and

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

C(1)—C(2)	1.397 (8)	C(2)—N(1)	1.481 (8)
C(2)—C(3)	1.399 (8)	C(4)—N(2)	1.490 (7)
C(3)—C(4)	1.366 (7)	N(1)—O(1)	1.213 (8)
C(4)—C(5)	1.373 (8)	N(1)—O(2)	1.158 (7)
C(5)—C(6)	1.356 (8)	N(2)—O(3)	1.212 (6)
C(6)—C(1)	1.372 (8)	N(2)—O(4)	1.237 (6)
C(1)—F(1)	1.336 (7)		
C(2)—C(1)—C(6)	120.0 (5)	C(5)—C(4)—N(2)	119.4 (6)
C(2)—C(1)—F(1)	120.1 (6)	C(4)—C(5)—C(6)	119.1 (6)
C(6)—C(1)—F(1)	119.8 (6)	C(5)—C(6)—C(1)	120.4 (6)
C(1)—C(2)—C(3)	120.2 (5)	C(2)—N(1)—O(1)	117.5 (7)
C(1)—C(2)—N(1)	122.4 (6)	C(2)—N(1)—O(2)	118.3 (7)
C(3)—C(2)—N(1)	117.4 (6)	O(1)—N(1)—O(2)	124.2 (7)
C(2)—C(3)—C(4)	116.9 (6)	C(4)—N(2)—O(3)	118.4 (6)
C(3)—C(4)—C(5)	123.4 (6)	C(4)—N(2)—O(4)	118.2 (6)
C(3)—C(4)—N(2)	117.2 (6)	O(3)—N(2)—O(4)	123.5 (6)

Related literature. Structure determinations on the chloro analogue have been published (Watson, 1960; Gopalakrishna, 1969; Takazawa, Ohba & Saito, 1989; Wilkins, Small & Gleghorn, 1990). The only published work on a structure involving F *ortho* to a nitro group in a benzene derivative is on 5-fluoro-2,4,6-trinitro-1,3-benzenediamine (Ammon, Bhattacharjee & Holden, 1982).

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$c \rightarrow a$). Final $R = 0.091$ for 593 observed reflections [$I > 2\sigma(I)$]. All dimensions are within the expected ranges.

Experimental. Colourless needle crystals obtained by recrystallization in methanol from the crude reaction product of diazotized (aqueous HCl and NaNO₂) 2,6-dimethylaniline and KCN/CuSO₄ in aqueous ammonium hydroxide solution (Haring, 1960). Crystal size 0.18 × 0.35 × 0.60 mm mounted about the b axis. Data collection on a Stoe STADI-2 diffractometer via variable-width ω scan. Lattice constants from axial reflections. Standard reflections $2k2$, no observed change in intensity. Background counts were 20s and a scan rate of 0.03333° s⁻¹ was applied with a width of $(1.5 + \sin\mu/\tan\theta)^\circ$. 1539 independent reflections measured up to a 2θ maximum of 50° of which 593 with $I > 2\sigma(I)$ were used in subsequent refinement. No absorption correction was made. Structure determined by direct methods using *SHELX76* (Sheldrick, 1976). H atoms were included in calculated positions; those in each methyl group were given a common thermal parameter and refined as a rigid group. Non-H atoms were refined anisotropically. 100 parameters were refined using full-matrix least-squares methods on F with a weighting scheme $w = 1/[\sigma^2(F) + 0.003F^2]$. Calculations were performed using *SHELX76* (Sheldrick, 1976) and some of our own programs on the Amdahl 5870 computer at the University of Reading. Final R value 0.091 ($wR = 0.095$). High R value due to broad and somewhat irregular peak shapes. Maximum Δ/σ 0.25. Maximum and minimum peaks in final difference Fourier map 0.28 and $-0.35 \text{ e } \text{Å}^{-3}$, respectively.

An *ORTEP* (Johnson, 1976) drawing of the molecule is given in Fig. 1 together with the atom numbering. Positional coordinates are given in Table 1 and bond distances and angles in Table 2.* Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV).

Related literature. This structure determination forms part of our studies of nitrile and isonitrile complexes of bivalent transition-metal halides (Drew, Dodd, Williamson & Willey, 1986). The structure of a tetragonal modification of benzonitrile at 198 K has been reported (Fauvet, Massaux & Chevalier, 1978).

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53370 (6 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Atomic coordinates ($\times 10^4$) with e.s.d.'s in parentheses

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

	x	y	z	$U_{eq}(\text{Å}^2 \times 10^3)$
C(1)	1210 (5)	5807 (8)	4971 (4)	83 (10)
C(2)	299 (5)	6126 (7)	3989 (5)	104 (10)
C(3)	-244 (5)	4687 (8)	3393 (5)	83 (10)
C(4)	82 (5)	3011 (9)	3736 (5)	82 (10)
C(5)	979 (5)	2711 (8)	4702 (5)	113 (11)
C(6)	1552 (5)	4082 (8)	5342 (5)	101 (10)
C(7)	1802 (5)	7310 (10)	5615 (5)	101 (11)
N(8)	2260 (6)	8482 (9)	6104 (5)	125 (12)
C(9)	-53 (6)	7997 (8)	3611 (5)	111 (12)
C(10)	2510 (6)	3790 (10)	6394 (5)	110 (11)

Table 2. Molecular dimensions: distances (Å) and angles (°)

C(1)—C(2)	1.416 (8)	C(3)—C(4)	1.374 (9)
C(1)—C(6)	1.422 (9)	C(4)—C(5)	1.391 (9)
C(1)—C(7)	1.468 (10)	C(5)—C(6)	1.383 (9)
C(2)—C(3)	1.387 (8)	C(6)—C(10)	1.502 (9)
C(2)—C(9)	1.530 (8)	C(7)—N(8)	1.136 (8)
C(2)—C(1)—C(6)	121.7 (5)	C(3)—C(4)—C(5)	120.4 (5)
C(2)—C(1)—C(7)	118.5 (5)	C(4)—C(5)—C(6)	121.1 (6)
C(6)—C(1)—C(7)	119.8 (5)	C(1)—C(6)—C(5)	117.6 (6)
C(1)—C(2)—C(3)	117.5 (5)	C(1)—C(6)—C(10)	120.3 (5)
C(1)—C(2)—C(9)	120.5 (5)	C(5)—C(6)—C(10)	122.1 (6)
C(3)—C(2)—C(9)	122.0 (5)	C(1)—C(7)—N(8)	179.1 (8)
C(2)—C(3)—C(4)	121.7 (5)		

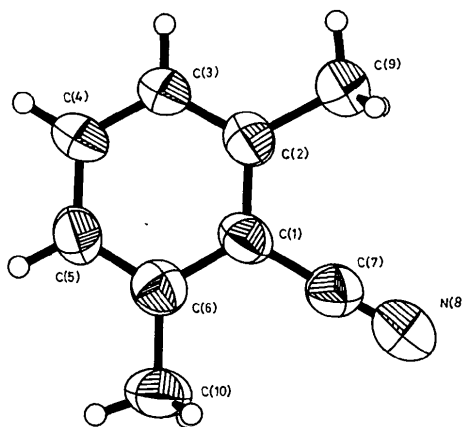


Fig. 1. View of the molecule showing the atom-numbering scheme. Thermal ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

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