

scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). Table 1 shows the atomic coordinates, Table 2 lists bond distances and angles, and the molecule is plotted in Fig. 1.*

Related literature. A number of macrocyclic trichothecenes have been reported. These include Verrucaric acid (McPhail & Sim, 1966), Verrucaric acid B (Breitenstein, Tamm, Arnold & Clardy, 1979), Baccharin (Kupchan, Jarvis, Dailey, Bright, Bryan & Yoshikazu, 1976) and Roridan A (Jarvis, Midiwo, Flippen-Anderson & Mazzola, 1982). The structures of Myrotoxin A and C (Jarvis, Cömezoglu, Lee, Flippen-Anderson, Gilardi & George, 1986) which were produced from the same *myrothecium roridum* culture as Myrotoxin B hydrate share a nearly identical conformation for the trichothecene ring. The

* 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 53301 (18pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

conformation of the common portion of the macrocyclic ring has its largest differences in the area of the tetrahydropyran ring due to differences in hydrogen bonding and packing.

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1-Fluoro-2,4-dinitrobenzene

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Abstract. $C_6H_3FN_2O_4$, $M_r = 186.0$, orthorhombic, $P2_12_12_1$, $a = 6.210$ (5), $b = 9.45$ (1), $c = 12.85$ (1) Å, $V = 754.1$ Å³, $Z = 4$, $D_x = 1.638$, $D_m = 1.63$ g cm⁻³, $F(000) = 376$, $\lambda(\text{Mo } K\alpha) = 0.7107$ Å, $\mu = 0.106$ mm⁻¹, $T = 293$ K. Diffractometer data, $R = 0.057$ for 611 unique observed reflexions. The nitro group *ortho* to F is twisted 16.0 (7)° relative to the plane of the benzene ring giving $F \cdots O$ of 2.575 (7) Å; the *para* nitro group is twisted through 8.4 (7)°.

Experimental. Commercial sample, recrystallized from ethanol, pale yellow prisms, melting point 299 K, density by flotation, crystal size $0.5 \times 0.4 \times 0.4$ mm. Crystal in capillary tube on STADI-2 two-circle diffractometer, cell dimensions from setting angles of 24 reflexions in the range $20 < 2\theta < 40^\circ$. Intensities for layers $0kl$ to $7kl$; k , 0 to 10; l , 0 to 17; standard every 20 reflexions, maximum $\sin\theta/\lambda$

0.70 Å⁻¹, measured on the STADI-2, variable ω scan, $2\theta'$ fixed, stationary background count. Lp corrections but no absorption correction, 1185 unique measured reflexions of which 611 with $I >$

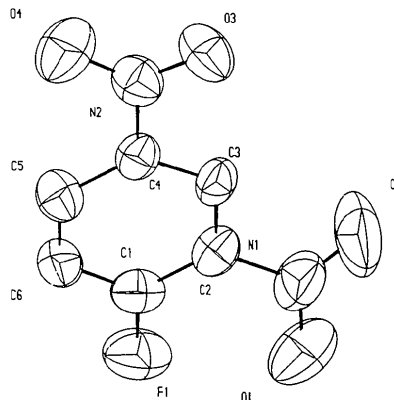


Fig. 1. Molecule of 1-fluoro-2,4-dinitrobenzene, showing atomic labelling and 50% thermal ellipsoids.

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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, $F(000) = 560$, $D_x = 1.14 \text{ g cm}^{-3}$, $Z = 8$, $\text{Mo K}\alpha$ 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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