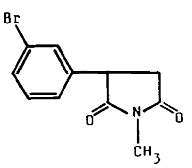
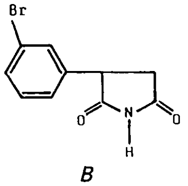
compound (*A*) is comparable to the activity of *m*-Br-phenylsuccinimide (*B*), a clinically used anticonvulsant (LEFADOL) (Lange *et al.*, 1966). This structure was investigated because of the very poor quality of monocrystals obtainable for LEFADOL.



A



B

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Structure of 2-Amino-5-methylisophthalonitrile

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Abstract. $C_9H_7N_3$, $M_r = 157{\cdot}2$, monoclinic, $P2_1/c$, $a = 7{\cdot}145\,(8)$, $b = 10{\cdot}866\,(5)$, $c = 11{\cdot}006\,(6)$ Å, $\beta = 107{\cdot}53\,(6)°$, $V = 814{\cdot}8$ Å^3, $Z = 4$, $D_x = 1{\cdot}281$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71069$ Å, $\mu = 0{\cdot}76$ cm^{-1}, $F(000) = 328$, $T = 293$ K, $R = 0{\cdot}048$ for 1023 observed reflections. The reaction of α,β-unsaturated aldehydes with malononitrile is a synthetic method leading to 2-alkoxy-3-cyanopyridines. In this reaction a minor product is also obtained having an isophthalonitrilic structure. Thus, the title compound comes from the reaction between methacrolein and malononitrile. The X-ray determination confirms the chemical structure. The amino group evenly releases electronic charge towards both nitrile groups. Bond distances, as well as NMR and IR data, are in agreement with this assumption.

Experimental. In the context of a study on the reaction between α,β-unsaturated aldehydes with malononitrile, the title compound was obtained in low yield as a side product. After chromatographic separation, single crystals were obtained by slow evaporation from a hexane solution. A suitable prismatic single crystal *ca* 0·5 × 0·4 × 0·4 mm was moun-

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Table 1. *Atomic coordinates and equivalent isotropic temperature factors* (Å^2) *with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{8}{3}\pi^2 \textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	B_{eq}
C1	0·2061 (3)	0·1531 (2)	0·5081 (2)	4·12 (6)
C2	0·3630 (3)	−0·0647 (2)	0·6188 (2)	4·49 (6)
N3	0·0916 (3)	0·0556 (2)	0·3024 (2)	4·76 (5)
C4	0·3054 (3)	0·1469 (2)	0·6368 (2)	4·50 (6)
C5	0·1818 (3)	0·0489 (2)	0·4286 (2)	3·93 (6)
C6	0·2646 (3)	−0·0610 (2)	0·4900 (2)	4·08 (6)
C7	0·4986 (5)	0·0331 (4)	0·8345 (3)	5·98 (9)
C8	0·3882 (3)	0·0386 (2)	0·6952 (2)	4·60 (6)
N9	0·0621 (4)	0·3568 (2)	0·4048 (2)	6·64 (9)
N10	0·2196 (4)	−0.2584 (2)	0·3569 (2)	6·24 (8)
C11	0·1251 (4)	0·2672 (2)	0·4525 (2)	4·78 (6)
C12	0·2416 (3)	−0.1708 (2)	0·4166 (2)	4·52 (6)

Table 2. *Bond lengths* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

C1—C4	1·382 (3)	C4—C8	1·385 (3)
C1—C5	1·409 (3)	C5—C6	1·411 (3)
C1—C11	1·426 (3)	C6—C12	1·422 (3)
C2—C6	1·381 (3)	C7—C8	1·499 (3)
C2—C8	1·382 (3)	N9—C11	1·133 (3)
N3—C5	1·346 (3)	N10—C12	1·140 (3)
C5—C1—C11	118·3 (3)	C2—C6—C5	121·8 (4)
C4—C1—C11	119·9 (4)	C5—C6—C12	118·6 (3)
C4—C1—C5	121·8 (5)	C2—C6—C12	119·6 (5)
C6—C2—C8	122·3 (5)	C4—C8—C7	121·9 (6)
C1—C4—C8	122·2 (4)	C2—C8—C7	121.4 (6)
C1—C5—N3	121·9 (6)	C2—C8—C4	116·7 (3)
N3—C5—C6	122·7 (4)	C1—C11—N9	177·7 (4)
C1—C5—C6	115·3 (3)	C6—C12—N10	178·7 (6)

ted on an Enraf–Nonius CAD-4 diffractometer using graphite-monochromatized Mo *Kα* radiation; lattice parameters from a least-squares fit of 25 reflections up to $2\theta = 34°$. Three standard reflections monitored every 100 measurements; no significant change in intensity. 1615 reflections measured with an $\omega/2\theta$ scan. 1444 unique of which 1023 with $I \geq 2{\cdot}5\sigma(I)$ were used in the refinement. Lorentz and polarization corrections were applied but no absorption or extinction corrections were made. 2θ limit = 50°. Index range h +/−8, k 0/13, l 0/13.

The structure was solved by direct methods using *MULTAN*11/84 (Main, Germain & Woolfson, 1984). All non-H atoms located from an *E* map prepared using the phase set with the highest figure of merit. The refinement was performed by full-matrix least squares on *F* using *SHELX*76 (Sheldrick, 1976). H atoms found in subsequent difference Fourier maps and refined with individual isotropic temperature factors. 138 parameters refined. Final $R = 0{\cdot}048$, $wR = 0{\cdot}058$, $w = 1/[\sigma^2(F) + 4{\cdot}9 \times 10^{-3}F^2]$; maximum shift/e.s.d. = 0·015; maximum and minimum heights in final difference Fourier synthesis 0·15 and −0·20 e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). Table 1 presents the final atomic coordinates and equivalent isotropic temperature factors for the 12 non-H atoms.* Interatomic distances and angles are shown in Table 2. Fig.1 shows a view of the molecule with atom numbering.

Related literature. A synthesis of pyridines based on the condensation of malononitrile with *α,β*-unsaturated aldehydes in a basic alcoholic medium has been reported by Victory, Borrell & Vidal-Ferran (1991). The title compound has been previously obtained by another synthetic method (Detzer & Burkhard, 1987). Few structural data of single isophthalonitriles have been reported (Carter, Turley, & Boer, 1972; Britton, 1981; Bel'skii, Zviedre, Belyakov, Guttsait & Gudrinietse, 1985).

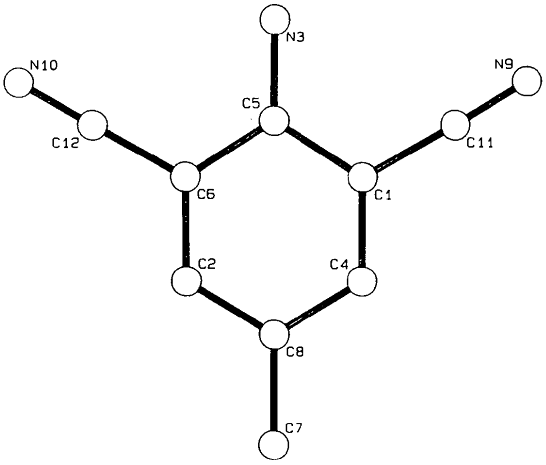

Fig. 1. View of the molecule with the atom-numbering scheme (*PC-PLUTO*; Schmid & Brueggemann, 1990).

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* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54467 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HE0024]