angles at C(1) [125·4 (7)°] and C(4) [123·4 (7)°] are significantly larger than the remainder (117·8° av.), as often observed when nitro or diazo groups are attached to a benzene ring. The title compound clearly belongs to the 'aromatic' class of diazo compounds.

In benzenediazonium tetrafluoroborate where the anions are ordered, each N atom has four contacts to F in the range 2·84–3·10 Å. The shortest distance from F to azo N in the present structure is N(8)···F(15*A*), 2·621 (9) Å, significantly shorter than the sum of van der Waals radii (2·85 Å). N(8)···F(13) is 2·914 (9) Å. N(7) has no contacts to F under 3·1 Å. F(14*A*) is close to the nitro group, 2·663 (10) Å to N(9) and 2·86 Å to O(10), O(11).

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Structure of 8-Dimethylamino-1-naphthonitrile

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Abstract. $C_{13}H_{12}N_2$, $M_r = 196{\cdot}25$, monoclinic, Pc, $a = 8{\cdot}786\,(3)$, $b = 9{\cdot}341\,(4)$, $c = 7{\cdot}071\,(3)$ Å, $\beta = 110{\cdot}24\,(3)°$, $V = 544{\cdot}5$ Å^3, $Z = 2$, $D_x = 1{\cdot}197$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}0672$ mm^{-1}, $F(000) = 208$, $T = 293\,(1)$ K, $R = 0{\cdot}0708$ for 949 observed reflections with $I > 3\sigma(I)$. As a result of the substituents on the C(1) and C(8) atoms, the naphthyl moiety is twisted with deviations of these atoms of $-0{\cdot}071$ and 0·099 Å, respectively, from the least-squares plane of the naphthalene ring, the C—C≡N angle in the nitrile group is 171·2 (4)° and the amine N atom is 0·361 (3) Å from the plane of its three bonded C atoms.

Experimental. 1,8-Naphthoic anhydride was converted to 8-bromo-1-naphthoic acid (Bailey, Card & Shechter, 1983) which was reacted with concentrated sulfuric acid and sodium azide to yield 8-bromo-1-naphthylamine. The amine was methylated and then converted to the title compound by the procedure reported by Whitaker & Snyder (1970). The product was recrystallized from hexane by slow evaporation at room temperature. A crystal of approximate dimensions 0·17 × 0·15 × 0·45 mm was cut from a long needle and used for data collection on an Enraf–Nonius CAD-4 diffractometer with graphite-monochromatized Mo $K\alpha$ radiation. The cell constants and orientation matrix were determined by least-squares refinement of the setting angles of 21 reflections in the 10–15° range. Intensity data were collected in the range $2 < \theta < 27°$ using the ω–2θ scan method and variable scan speed. The intensities of two standard reflections, monitored at regular intervals, did not show significant variation. 1758 reflections measured, 1650 unique ($R_{\text{int}} = 0{\cdot}007$) ($h\,0\rightarrow12$, $k\,0\rightarrow12$, $l\,-9\rightarrow9$) of which 949 with $I > 3\sigma(I)$ were considered observed. Data were corrected for Lorentz, polarization and absorption effects (North, Phillips & Mathews, 1968); the max. and min. correction factors were 0·9986 and 0·9092, respectively.

The structure was solved by direct methods using *MULTAN*82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) and refined by full-matrix least-squares calculations of F's. H atoms were located from a difference map and included in the refinement with the overall isotropic temperature factor $B_{\text{iso}} = 5{\cdot}0$ Å^2; C and N had anisotropic temperature factors. The refinement converged completely with $R = 0{\cdot}0708$ and $wR = 0{\cdot}0932$, where $w = [\sigma^2(F_o) + (0{\cdot}080F_o)^2]^{-1}$; max. shift/e.s.d. in the last cycle of refinement was < 0·07 and goodness of fit, $S = 1{\cdot}723$. A final difference map was devoid of significant features with $\Delta\rho$ in the range $-0{\cdot}35$ to $0{\cdot}32$ e Å^{-3}. Scattering factors used in the calcula-

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Table 1. *Final fractional coordinates and equivalent isotropic thermal parameters* (Å^2) *with e.s.d.'s in parentheses*

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

	x	y	z	B_{eq}
N1	0·1387	0·7897 (5)	0·6250	6·07 (8)
N2	0·1879 (4)	0·7023 (4)	0·2095 (5)	4·39 (7)
C1	0·4200 (4)	0·8075 (4)	0·5847 (5)	4·03 (7)
C2	0·5314 (5)	0·8730 (6)	0·7544 (6)	5·1 (1)
C3	0·6944 (6)	0·8833 (6)	0·7702 (8)	6·1 (1)
C4	0·7462 (6)	0·8203 (6)	0·6313 (8)	5·7 (1)
C5	0·6936 (5)	0·6806 (6)	0·3151 (7)	5·7 (1)
C6	0·5874 (6)	0·6125 (6)	0·1581 (7)	6·5 (1)
C7	0·4182 (6)	0·6181 (5)	0·1191 (6)	5·6 (1)
C8	0·3571 (5)	0·6888 (4)	0·2472 (5)	4·20 (8)
C9	0·4662 (4)	0·7499 (4)	0·4277 (6)	3·85 (7)
C10	0·6358 (5)	0·7521 (4)	0·4580 (6)	4·47 (8)
C11	0·2573 (5)	0·7932 (5)	0·5933 (6)	4·49 (7)
C12	0·0789 (7)	0·5990 (6)	0·0753 (7)	5·8 (1)
C13	0·1262 (6)	0·8480 (6)	0·1555 (7)	5·3 (1)

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

N1—C11	1.140 (5)	C3—C4	1·352 (9)
N2—C8	1·422 (6)	C4—C10	1·424 (6)
N2—C12	1·456 (6)	C5—C6	1·339 (6)
N2—C13	1·467 (6)	C5—C10	1·442 (8)
C1—C2	1·400 (5)	C6—C7	1·415 (8)
C1—C9	1·413 (6)	C7—C8	1·372 (7)
C1—C11	1·458 (6)	C8—C9	1·424 (5)
C2—C3	1·400 (8)	C9—C10	1·430 (6)

C8—N2—C12	118·3 (4)	C6—C7—C8	120·9 (4)
C8—N2—C13	113·5 (4)	N2—C8—C7	122·8 (3)
C12—N2—C13	110·2 (3)	N2—C8—C9	117·9 (4)
C2—C1—C9	122·3 (4)	C7—C8—C9	119·3 (4)
C2—C1—C11	114·1 (4)	C1—C9—C8	124·7 (4)
C9—C1—C11	123·4 (3)	C1—C9—C10	116·4 (3)
C1—C2—C3	119·4 (5)	C8—C9—C10	119·0 (4)
C2—C3—C4	120·3 (5)	C4—C10—C5	120·7 (5)
C3—C4—C10	121·4 (5)	C4—C10—C9	120·0 (4)
C6—C5—C10	119·2 (5)	C5—C10—C9	119·3 (3)
C5—C6—C7	121·9 (5)	N1—C11—C1	170·9 (4)

tions were taken from Cromer & Mann (1968) and Stewart, Davidson & Simpson (1965). The absolute structure was not determined. Computer programs used in this study were from the Enraf–Nonius *Structure Determination Package* (B. A. Frenz & Associates Inc., 1985) and *ORTEP*II (Johnson, 1976).

Final fractional coordinates and equivalent isotropic thermal parameters with e.s.d.'s are listed in Table 1.* Table 2 contains bond lengths and bond angles. Fig. 1 shows the molecular structure of the title compound. Fig. 2 is a stereoview of the unit-cell packing.

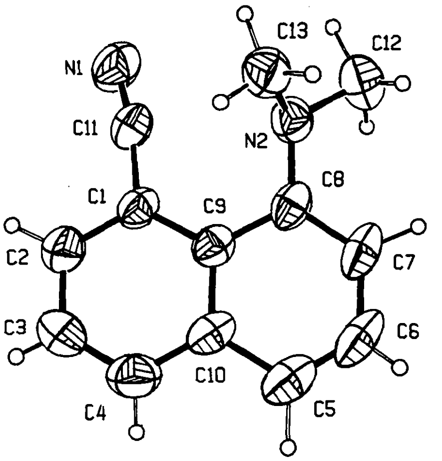

Fig. 1. *ORTEP* (Johnson, 1976) drawing of 8-dimethylamino-1-naphthonitrile showing the crystallographic numbering scheme.

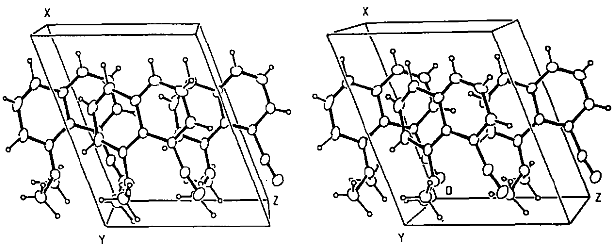

Fig. 2. Stereoview of the unit-cell packing.

Related literature. 8-Methoxy- and 8-nitronaphthonitrile (Procter, Britton & Dunitz, 1981); *N,N*-dimethyl-8-nitronaphthaleneamine (Egli, Wallis & Dunitz, 1986).

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* Lists of structure amplitudes, anisotropic temperature factors, least-squares-planes data and molecular dimensions involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52525 (15 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.