(Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978). All the H atoms found from difference synthesis. Non-H atoms refined with anisotropic thermal parameters, and H atoms with isotropic thermal parameters. $\sum w||F_o| - |F_c||^2$ minimized; $w^{-1} = \sigma^2(|F_o|) + (0{\cdot}015|F_o|)^2$. Final $R = 0{\cdot}039$, $wR = 0{\cdot}053$, $S = 1{\cdot}92$ for 1187 unique reflections.* $R_{int} = 0{\cdot}008$. $\Delta/\sigma < 0{\cdot}4$, $-0{\cdot}24 < \Delta\rho < 0{\cdot}17$ e Å^{-3}. Complex neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974); Universal Crystallographic Computation Program System *UNICS*III (Sakurai & Kobayashi, 1979). Final atomic coordinates are given in Table 1, and bond lengths and angles in Table 2.

Related literature. Two kinds of orthorhombic crystals of *o*-aminobenzoic acid grow in different conditions (Brown, 1968). Brown (1968) and Brown & Ehrenberg (1985) reported a lower-temperature form of the compound which contains a zwitterion, and Boone, Derissen & Schoone (1977) reported a higher-temperature form. The hydrogen-bonding scheme in the present crystal (Fig. 1) is almost the same as that in the other modifications. The structures of *m*- (Voogd, Verzijl & Duisenberg, 1980) and *p*-aminobenzoic acid (Lai & Marsh, 1967) have also been determined.

* Lists of structure factors, anisotropic thermal parameters, atomic parameters for H atoms, bond lengths and bond angles involving H atoms and distances from the least-squares plane through the benzene ring have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43242 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

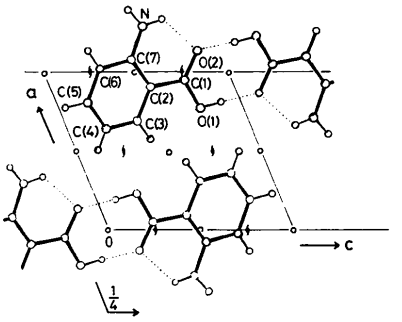

Fig. 1. A partial projection of the structure along **b**. Dotted lines indicate hydrogen bonds.

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N,N'-Dimethyl-*N,N'*-ethylenebis(nicotinamide)

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Abstract. $C_{16}H_{18}N_4O_2$, $M_r = 298{\cdot}4$, monoclinic, $P2_1/c$, $a = 8{\cdot}469$ (2), $b = 9{\cdot}727$ (3), $c = 9{\cdot}174$ (4) Å, $\beta = 92{\cdot}00$ (3)°, $V = 755{\cdot}3$ (8) Å^3, $Z = 2$, $D_x = 1{\cdot}312$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 0{\cdot}84$ cm^{-1}, $F(000) = 316$, $T = 297$ K, $R = 0{\cdot}041$ for 1391 observations (of 2193 unique data). The centrosymmetric molecule has a conformation in the crystal very similar to that observed in the phenyl analog, *N,N'*-dimethyl-*N,N'*-dibenzoylethylenediamine. The *N*-methyl group is oriented *syn* to the carboxyl group [O—C(3)—N(1)—C(2) torsion angle 2·4 (2)°], and the pyridine is twisted out of the carboxamide plane by 71·8 (2)° [torsion angle C(8)—C(4)—C(3)—O]. Pyridine C—C distances range from 1·368 (2) to 1·381 (1) Å, pyridine C—N lengths are 1·332 (2) and 1·338 (2) Å, and the central C—N bond of the amide linkage has length 1·342 (1) Å.

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Table 1. *Coordinates and isotropic thermal parameters* (Å²)

$B_{eq} = \frac{1}{3}(a^2a^{*2}B_{11} + B_{22} + c^2c^{*2}B_{33} + aca^*c^*B_{13}\cos\beta)$.

	x	*y*	*z*	B_{eq} or *B*
O	0·8559 (1)	0·3765 (1)	1·1076 (1)	4·39 (2)
N(1)	0·9534 (1)	0·1888 (1)	0·9973 (1)	3·10 (2)
N(2)	0·4339 (1)	0·1244 (1)	1·1262 (2)	5·41 (3)
C(1)	0·9418 (1)	0·0442 (1)	0·9558 (1)	3·00 (2)
C(2)	1·0893 (2)	0·2652 (2)	0·9450 (2)	4·20 (3)
C(3)	0·8473 (1)	0·2533 (1)	1·0784 (1)	3·01 (3)
C(4)	0·7132 (1)	0·1696 (1)	1·1351 (1)	3·03 (2)
C(5)	0·7324 (2)	0·0810 (2)	1·2517 (2)	3·79 (3)
C(6)	0·6018 (2)	0·0151 (2)	1·3040 (2)	4·36 (3)
C(7)	0·4567 (2)	0·0393 (2)	1·2388 (2)	4·84 (4)
C(8)	0·5620 (2)	0·1874 (2)	1·0768 (2)	4·49 (3)
H(5)	0·831 (2)	0·068 (1)	1·296 (2)	4·1 (3)
H(6)	0·610 (2)	−0·048 (2)	1·385 (2)	5·1 (3)
H(7)	0·363 (2)	−0·003 (1)	1·273 (2)	4·8 (3)
H(8)	0·545 (2)	0·245 (2)	0·992 (2)	5·0 (4)
H(11)	0·832 (1)	0·012 (1)	0·967 (1)	3·0 (3)
H(12)	0·963 (1)	0·037 (1)	0·853 (1)	3·2 (3)
H(21)	1·102 (2)	0·255 (2)	0·838 (2)	8·9 (5)
H(22)	1·185 (2)	0·233 (2)	0·986 (2)	6·1 (4)
H(23)	1·080 (2)	0·359 (2)	0·959 (2)	6·3 (4)

Experimental. Colorless prisms by evaporation from 2:1 CH_2Cl_2/CCl_4, dimensions 0·32 × 0·40 × 0·48 mm. Space group from systematic absences *h*0*l* with *l* odd and 0*k*0 with *k* odd. Enraf–Nonius CAD-4 diffractometer with graphite monochromator and Mo *K*α radiation. Cell dimensions from setting angles of 25 reflections having $22 < 2\theta < 24°$. Data collection by ω–2θ scans designed for $I = 50\sigma(I)$, subject to 120 s max. scan time. Scan rates 0·39–4·0° min⁻¹. 2193 reflections having $1 < \theta < 30°$, $0 \le h \le 11$, $0 \le k \le 13$, $-12 \le l \le 12$ measured, corrected for background, Lorentz, polarization effects, absorption insignificant. Standard reflections (200, 020, 002), ±3·2% max. variation. Redundant 0*kl* and 0*k*$\bar{l}$ data averaged, $R_{int} = 0{\cdot}011$. Structure solved using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), refined by full-matrix least squares based on *F*, using data for which $I > 3\sigma(I)$, 802 unobserved reflections, $w = 4F_o^2[\sigma^2(I) + (0{\cdot}02F_o^2)^2]^{-1}$, with Enraf–Nonius *SDP* (Frenz & Okaya, 1980). Non-H atoms anisotropic; H atoms located by ΔF and refined isotropically. Final $R = 0{\cdot}041$ (0·085 all data), $wR = 0{\cdot}048$, $S = 2{\cdot}334$ for 137 variables, max. residual density 0·18, min. −0·12 e Å⁻³, max. shift $0{\cdot}04\sigma$ on final cycle, extinction coefficient 9 (3) $\times 10^{-7}$ $[|F_c| = |F_o|(1 + gI_c)]$. Atomic scattering factors of Cromer & Waber (1974). Atomic coordinates and equivalent isotropic thermal parameters in Table 1,* bond distances and angles in Table 2. Fig. 1 shows the atom-numbering scheme.

* Lists of anisotropic thermal parameters, structure-factor amplitudes and deviations from the pyridine best plane have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43179 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

O–C(3)	1·229 (1)	C(1)–C(1')	1·521 (2)
N(1)–C(1)	1·460 (1)	C(3)–C(4)	1·505 (1)
N(1)–C(2)	1·465 (1)	C(4)–C(5)	1·379 (1)
N(1)–C(3)	1·342 (1)	C(4)–C(8)	1·381 (1)
N(2)–C(7)	1·332 (2)	C(5)–C(6)	1·378 (1)
N(2)–C(8)	1·338 (2)	C(6)–C(7)	1·368 (2)
	C–H range 0·928 (15)–0·994 (17)		
C(1)–N(1)–C(2)	116·69 (8)	C(3)–C(4)–C(5)	122·44 (8)
C(1)–N(1)–C(3)	123·73 (7)	C(3)–C(4)–C(8)	119·94 (9)
C(2)–N(1)–C(3)	119·58 (8)	C(5)–C(4)–C(8)	117·46 (9)
C(7)–N(2)–C(8)	116·71 (10)	C(4)–C(5)–C(6)	119·09 (10)
N(1)–C(1)–C(1')	111·64 (10)	C(5)–C(6)–C(7)	119·14 (12)
O–C(3)–N(1)	122·77 (8)	N(2)–C(7)–C(6)	123·33 (10)
O–C(3)–C(4)	119·44 (8)	N(2)–C(8)–C(4)	124·27 (11)
N(1)–C(3)–C(4)	117·80 (8)		

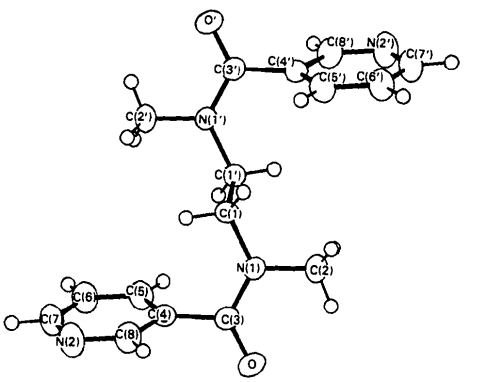

Fig. 1. Numbering scheme and thermal ellipsoids drawn at the 40% probability level. H atoms have arbitrary radius.

Related literature. Synthesis and evidence of various conformers in solution by VTNMR: (Newkome & Kawato, 1980); structure of *N,N'*-dimethyl-*N,N'*-dibenzoylethylenediamine, the phenyl analog: (Lepore, Ganis, Bombieri, Gilli & Montaudo, 1977); (*s*)-*N*-(α-methylbenzyl)nicotinamide: (Little & Morimoto, 1981).

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