Table 2. *Interatomic distances* (Å) *and bond angles* (°)

C(1)–F(1)	1·318 (5)	C(1)–F(2)	1·318 (5)
C(1)–F(3)	1·333 (5)	C(1)–C(2)	1·496 (6)
C(2)–Cl(1)	1·719 (4)	C(2)–C(3)	1·317 (5)
C(3)–C(4)	1·467 (5)	C(4)–C(5)	1·530 (5)
C(4)–C(7)	1·515 (5)	C(5)–C(6)	1·472 (5)
C(5)–C(7)	1·511 (6)	C(6)–O(1)	1·226 (4)
C(6)–O(2)	1·305 (5)	C(7)–C(8)	1·517 (5)
C(7)–C(9)	1·506 (6)		

F(1)–C(1)–F(2)	107·9 (4)	F(1)–C(1)–F(3)	106·7 (4)
F(2)–C(1)–F(3)	105·9 (4)	F(1)–C(1)–C(2)	112·0 (3)
F(2)–C(1)–C(2)	111·7 (4)	F(3)–C(1)–C(2)	112·3 (4)
Cl(1)–C(2)–C(1)	112·5 (3)	Cl(1)–C(2)–C(3)	123·5 (3)
C(1)–C(2)–C(3)	124·1 (4)	C(2)–C(3)–C(4)	125·7 (4)
C(3)–C(4)–C(5)	121·3 (3)	C(3)–C(4)–C(7)	122·3 (3)
C(5)–C(4)–C(7)	59·5 (2)	C(4)–C(5)–C(6)	121·2 (3)
C(4)–C(5)–C(7)	59·7 (3)	C(7)–C(5)–C(6)	124·6 (4)
C(5)–C(6)–O(1)	124·4 (4)	C(5)–C(6)–O(2)	112·2 (4)
O(1)–C(6)–O(2)	123·4 (4)	C(4)–C(7)–C(5)	60·7 (2)
C(4)–C(7)–C(8)	115·8 (3)	C(4)–C(7)–C(9)	120·6 (3)
C(5)–C(7)–C(8)	113·7 (3)	C(5)–C(7)–C(9)	121·1 (3)
C(8)–C(7)–C(9)	114·6 (3)		

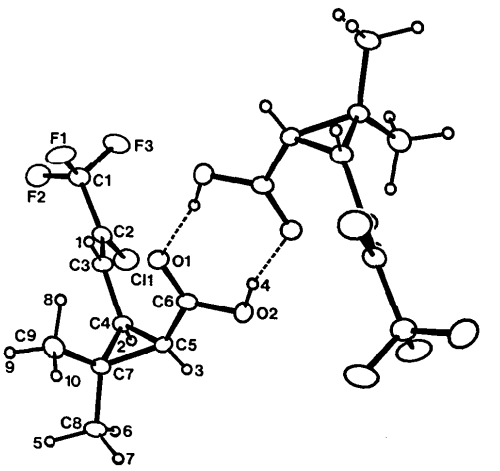

Fig. 1. Crystallographic numbering scheme for cyhalothric acid showing the association between centrosymmetrically related molecules (*ORTEP*, Johnson, 1971). Atoms otherwise not indicated are H atoms.

laboratory μ-VAX computer system. Atomic parameters given in Table 1, selected bond distances and angles in Table 2,* the numbering scheme used is shown in Fig. 1.

Related literature. Cyhalothric acid is an intermediate in the industrial preparation of the cyano(3-phenoxyphenyl)methyl ester of cyhalothric acid, cyhalothrin, one of the synthetic pyrethrins. The spectral and X-ray analyses reported here have shown that the *cis*-cyhalothric acid used in this preparation exists exclusively as the *Z* isomer.

The Australian Research Grants Scheme is thanked for support and Dr E. J. McGarry (ICI) is thanked for the gift of cyhalothric acid.

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and interatomic distances and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44260 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of *N*-[2-(Nitrooxy)ethyl]nicotinamide (SG 75)

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Abstract. $C_8H_9N_3O_4$, $M_r = 211{\cdot}18$, monoclinic, $P2_1/a$, $a = 9{\cdot}519$ (1), $b = 19{\cdot}498$ (2), $c = 5{\cdot}230$ (1) Å, $\beta = 102{\cdot}10(2)°$, $V = 954{\cdot}1$ Å^3, $Z = 4$, $D_x = 1{\cdot}478$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 9{\cdot}9$ cm^{-1}, $F(000) = 440$, $T = 298$ K, final $R = 0{\cdot}052$ for 1327 unique reflections [$F_o^2 > 2{\cdot}0\,\sigma(F_o^2)$]. The SG 75 molecule adopts a folded conformation, which is stabilized by intramolecular van der Waals contacts between the carbonyl O atom and the nitro group. Intermolecular H bonds and short contacts are observed.

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0108-2701/87/122460-03$01.50

Experimental. Colorless thin plates of SG 75 grown from methanol. Crystal size 0·20 × 0·12 × 0·02 mm, Enraf–Nonius CAD-4 κ-cradle diffractometer, Cu $K\alpha$ radiation, graphite monochromator, θ–2θ scan with scan speed 0·92–8·24° min^{-1} in θ, scan width (0·60 + 0·14tanθ)°. Range of indices, $-11 \le h \le 11$, $0 \le k \le 24$, $0 \le l \le 6$ ($2\theta < 150°$). Lattice parameters determined based on 25 2θ values ($21 < 2\theta \le 112°$). Variation of standard < 0·4%; 1954 reflections measured; 1327 observed reflections with $F_o^2 > 2{\cdot}0\sigma(F_o^2)$. Systematic absences $h0l$, h odd; $0k0$, k odd. No corrections for absorption. Structure solved by direct methods with *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). Refined by full-matrix least squares. The locations of H atoms were calculated stereochemically. Non-H atoms refined with anisotropic thermal parameters, and H atoms with isotropic thermal parameters (fixed at $B = 5{\cdot}0$ Å^2). $\sum w(|F_o| - |F_c|)^2$ minimized; $w = 1{\cdot}0$ for $F_o < 519{\cdot}5$, $w = (519{\cdot}5/F_o)^2$ for $F_o \ge 519{\cdot}5$. Final $R = 0{\cdot}052$, $wR = 0{\cdot}055$, $S = 4{\cdot}61$ for 173 variables, secondary-extinction factor $g = 2{\cdot}9\ (2) \times 10^{-6}$ [$|F_o| = |F_c|/(1 + gI_c)$]; $\Delta/\sigma \le 0{\cdot}09$, largest peak in final ΔF map 0·20 e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); programs: Enraf–Nonius *SDP* (Frenz, 1984), *ORTEP*II (Johnson, 1976). The structure of the SG 75 molecule is shown in Fig. 1, and Fig. 2 shows a packing diagram of the molecule. Positional parameters and equivalent values of the anisotropic temperature factors are given in Table 1; bond distances and angles are listed in Table 2.*

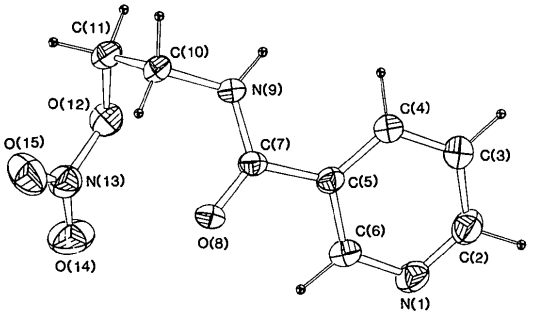

Fig. 1. A perspective view of the molecule with the numbering scheme.

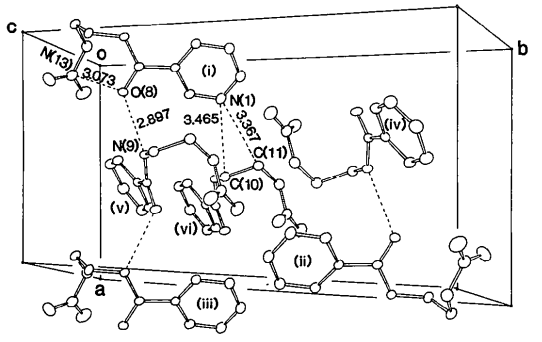

Fig. 2. Packing view of SG 75. O···H–N hydrogen bonds, intra- and intermolecular short contacts are indicated by broken lines. Symmetry codes: (i) $x-1, y, z$; (ii) $2-x, 1-y, 1-z$; (iii) x, y, z; (iv) $1\frac{1}{2}-x, \frac{1}{2}+y, 1-z$; (v) $x-\frac{1}{2}, \frac{1}{2}-y, z$; (vi) $x-\frac{1}{2}, \frac{1}{2}-y, z-1$.

Table 1. *Final fractional coordinates and equivalent isotropic temperature factors for non-*H *atoms with e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j$

	x	y	z	B_{eq}(Å^2)
N(1)	1·1845 (3)	0·3557 (2)	0·1240 (5)	3·88 (6)
C(2)	1·0913 (4)	0·4060 (2)	0·1316 (7)	4·21 (8)
C(3)	0·9952 (4)	0·4066 (2)	0·2965 (8)	4·25 (8)
C(4)	0·9972 (4)	0·3525 (2)	0·4688 (7)	3·43 (7)
C(5)	1·0950 (3)	0·3001 (2)	0·4695 (6)	2·56 (6)
C(6)	1·1850 (3)	0·3039 (2)	0·2911 (6)	3·24 (7)
C(7)	1·1136 (3)	0·2402 (2)	0·6512 (6)	2·66 (6)
O(8)	1·2277 (2)	0·2078 (1)	0·6970 (5)	3·40 (5)
N(9)	1·0025 (3)	0·2235 (1)	0·7580 (5)	2·86 (5)
C(10)	1·0098 (4)	0·1661 (2)	0·9368 (6)	3·18 (7)
C(11)	0·9437 (4)	0·1017 (2)	0·8028 (7)	3·57 (7)
O(12)	1·0042 (3)	0·0846 (1)	0·5765 (5)	3·79 (5)
N(13)	1·1400 (3)	0·0560 (2)	0·6363 (6)	4·08 (7)
O(14)	1·1931 (3)	0·0481 (2)	0·4501 (6)	6·35 (7)
O(15)	1·1895 (3)	0·0410 (2)	0·8603 (6)	5·57 (7)

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

N(1)–C(2)	1·328 (5)	C(7)–N(9)	1·337 (4)
N(1)–C(6)	1·335 (5)	N(9)–C(10)	1·450 (4)
C(2)–C(3)	1·383 (6)	C(10)–C(11)	1·510 (5)
C(3)–C(4)	1·385 (5)	C(11)–O(12)	1·459 (5)
C(4)–C(5)	1·381 (5)	O(12)–N(13)	1·382 (4)
C(5)–C(6)	1·394 (5)	N(13)–O(14)	1·198 (5)
C(5)–C(7)	1·493 (4)	N(13)–O(15)	1·204 (4)
C(7)–O(8)	1·236 (4)		

C(2)–N(1)–C(6)	116·7 (3)	C(5)–C(7)–N(9)	117·3 (3)
N(1)–C(2)–C(3)	124·0 (4)	O(8)–C(7)–N(9)	122·3 (3)
C(2)–C(3)–C(4)	118·6 (4)	C(7)–N(9)–C(10)	121·5 (3)
C(3)–C(4)–C(5)	118·8 (4)	N(9)–C(10)–C(11)	112·5 (3)
C(4)–C(5)–C(6)	117·9 (3)	C(10)–C(11)–O(12)	111·7 (3)
C(4)–C(5)–C(7)	124·8 (3)	C(11)–O(12)–N(13)	114·7 (2)
C(6)–C(5)–C(7)	117·4 (3)	O(12)–N(13)–O(14)	113·7 (3)
N(1)–C(6)–C(5)	124·0 (3)	O(12)–N(13)–O(15)	118·4 (3)
C(5)–C(7)–O(8)	120·4 (3)	O(14)–N(13)–O(15)	127·9 (3)

Related literature. SG 75 is an antiangional agent (Nicorandil: Sakai, Akima, Hinohara & Obatake,

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44296 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of Propionanilide Derivative AN132

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Abstract. 3-{*N*-[2''-(*N'*,*N'*-Diisopropylamino)]ethylamino}-2',6'-dimethylpropionanilide (AN132), $C_{19}H_{33}NO_3$, $M_r = 319{\cdot}49$, orthorhombic, *Pbca*, $a = 21{\cdot}628\ (2)$, $b = 22{\cdot}542\ (2)$, $c = 8{\cdot}326\ (1)$ Å, $V = 4059{\cdot}2$ Å^3, $Z = 8$, $D_x = 1{\cdot}046$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 4{\cdot}75$ cm^{-1}, $F(000) = 1408$, $T = 298$ K, final $R = 0{\cdot}054$ for 1155 unique reflections [$F_o^2 > 2\sigma(F_o^2)$]. The amide group, connecting a benzene ring and a zigzag chain, is approximately perpendicular to both best planes. The carbonyl O atom forms intermolecular H bonds with two –NH groups in an adjacent molecule.

Experimental. Colorless needles of AN132 grew from isopropyl ether. Crystal size 0·43 × 0·13 × 0·05 mm, Enraf–Nonius CAD-4 κ-cradle diffractometer, Cu $K\alpha$ radiation, graphite monochromator, θ–2θ scan with scan speed 2·75–4·12° min^{-1} in θ, scan width (0·55 + 0·14tanθ)°. Range of indices $0 \le h \le 26$, $0 \le k \le 27$, $0 \le l \le 10$ ($2\theta < 140°$). Lattice constants determined based on 25 2θ values ($16 < 2\theta < 49°$). Variation of standard < 4·1%; 3839 unique reflections measured; 1155 observed reflections with $F_o^2 > 2\sigma(F_o^2)$. Systematic absences 0*kl*, *k* odd; *h*0*l*, *l* odd; *hk*0, *h* odd. No corrections for absorption. Structure solved by direct methods with *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). Refined by full-matrix least squares. The locations of H atoms were calculated stereochemically, except for that of H(11) found from difference Fourier map. Non-H atoms refined with anisotropic thermal parameters, and H atoms with isotropic thermal parameters (B = 5·0 Å^2: fixed). $\sum w(|F_o| - |F_c|)^2$ minimized; $w = 1{\cdot}0$ for $F_o < 472{\cdot}6$, $w = (472{\cdot}6/F_o)^2$ for $F_o \ge 472{\cdot}6$. Final $R = 0{\cdot}054$, $wR = 0{\cdot}047$, $S = 3{\cdot}90$ for 341 variables, secondary-extinction factor (g) 1·3 (1) × 10^{-7} [$|F_o| = |F_c|/(1+gI_c)$]; $\Delta/\sigma < 1{\cdot}1$, largest peak in final ΔF map +0·16 e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); programs: Enraf–Nonius *SDP* (Frenz, 1984), *ORTEP*II (Johnson, 1976). The structure of AN132 is shown in Fig. 1; a projection of the crystal structure is shown in Fig. 2. Positional parameters and equivalent values of the anisotropic temperature factors are given

Table 1. *Final fractional coordinates and equivalent isotropic temperature factors for non*-H *atoms with e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i\mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
C(1)	0·4098 (2)	0·2546 (3)	0·3756 (7)	4·6 (1)
C(2)	0·4506 (3)	0·2117 (3)	0·4271 (8)	6·4 (2)
C(3)	0·5044 (3)	0·2297 (4)	0·505 (1)	9·5 (2)
C(4)	0·5160 (3)	0·2882 (4)	0·5292 (9)	10·0 (3)
C(5)	0·4766 (3)	0·3296 (3)	0·4778 (8)	7·7 (2)
C(6)	0·4217 (3)	0·3129 (3)	0·4021 (6)	5·3 (2)
N(7)	0·3558 (2)	0·2369 (2)	0·2931 (5)	4·9 (1)
C(8)	0·3080 (3)	0·2095 (2)	0·3615 (7)	4·4 (1)
C(9)	0·2534 (3)	0·1959 (2)	0·2553 (7)	5·3 (1)
C(10)	0·1988 (3)	0·2320 (3)	0·3034 (7)	5·4 (2)
N(11)	0·2135 (2)	0·2942 (2)	0·3032 (5)	5·1 (1)
C(12)	0·1610 (3)	0·3327 (3)	0·3345 (7)	5·6 (2)
C(13)	0·1806 (3)	0·3969 (3)	0·3355 (8)	6·2 (2)
N(14)	0·1290 (2)	0·4361 (2)	0·3687 (6)	5·5 (1)
C(15)	0·0925 (3)	0·4509 (3)	0·2314 (9)	8·4 (2)
C(16)	0·1133 (5)	0·4908 (7)	0·114 (1)	20·7 (5)
C(17)	0·1404 (3)	0·4835 (3)	0·4797 (9)	8·4 (2)
C(18)	0·1414 (6)	0·4612 (4)	0·640 (1)	16·7 (4)
C(19)	0·1991 (4)	0·5185 (4)	0·457 (2)	17·3 (4)
C(20)	0·4417 (3)	0·1480 (3)	0·397 (1)	9·7 (2)
C(21)	0·3762 (3)	0·3596 (3)	0·3514 (8)	7·3 (2)
O(22)	0·3078 (2)	0·1965 (2)	0·5051 (4)	5·32 (9)
C(23)	0·0265 (4)	0·4675 (3)	0·275 (1)	9·8 (2)

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