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Structures of Isomeric N-(5-Methyl-2-aminobenzhydrylidene)amino-5-norbornene-2,3-*exo*-dicarboximide and N-(5-Methyl-2-aminobenzhydrylidene)amino-5-norbornene-2,3-*endo*-dicarboximide

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Abstract. $C_{23}H_{21}N_3O_2$ (*exo* isomer), $M_r = 371 \cdot 44$, monoclinic, $P2_1/n$, $a = 15 \cdot 593$ (14), $b = 11 \cdot 206$ (7), $c = 10 \cdot 808$ (7) Å, $\gamma = 96 \cdot 72$ (2)°, $V = 1875 \cdot 6$ (2·4) Å^3, $Z = 4$, $D_x = 1 \cdot 315$ (4) Mg m^{-3}, $\lambda(\text{Cu } K\alpha) = 1 \cdot 5418$ Å, $\mu = 0 \cdot 551$ mm^{-1}, $F(000) = 784$, $T = 293$ K, $R = 0 \cdot 056$ for 2801 observed reflections. $C_{23}H_{21}N_3O_2$ (*endo* isomer), $M_r = 371 \cdot 44$, monoclinic, $P2_1/n$, $a = 15 \cdot 065$ (15), $b = 11 \cdot 560$ (12), $c = 10 \cdot 720$ (10) Å, $\gamma = 94 \cdot 53$ (2)°, $V = 1861 \cdot 1$ (3·2) Å^3, $Z = 4$, $D_x = 1 \cdot 325$ (4) Mg m^{-3}, $\lambda(\text{Cu } K\alpha) = 1 \cdot 5418$ Å, $\mu = 0 \cdot 551$ mm^{-1}, $F(000) = 784$, $T = 293$ K, $R = 0 \cdot 055$ for 2804 observed reflections. Both *exo* and *endo* isomers possess a *cis*-conformation for the *o*-amino-phenyl ring, stabilized by strong intramolecular NH$\cdots$N bonds. The crystal structures of the two isomers are similar. The molecules in the crystal are linked in spirals around the screw axes. The spirals are connected by van der Waals interactions.

Introduction. It is known that *o*-acylaniline and norbornene hydrazone derivatives, besides being biologically active by themselves, are used to obtain other compounds possessing psychotropic, anticonvulsant and antimicrobic activity (Minoru, Morio & Hiroyuki, 1974; Minoru, Morio, Hiroyuki & Yasuo, 1974; Tasihiko & Syundzi, 1971). Therefore, the combination of both *o*-aminophenyl and norbornene fragments in the same molecule is potentially interesting. At the same time, the opportunity arises of studying the influence of the conformational peculiarities of these compounds on their biological activity. Accordingly, by boiling equimolecular quantities of 5-methyl-2-amino-benzophenone hydrazone (I) with 5-norbornene-2,3-*exo*- (II) or 5-norbornene-2,3-*endo*-dicarboxylic anhyd-

rides (III) in xylene we have prepared isomeric N-(5-methyl-2-aminobenzhydrylidene)amino-5-norbornene-2,3-*exo*- (IV) and *endo*-dicarboximide (V) (Andronati, Yavorsky, Bondarev, Salakov, Zakolodyajnaya & Terentev, 1985).
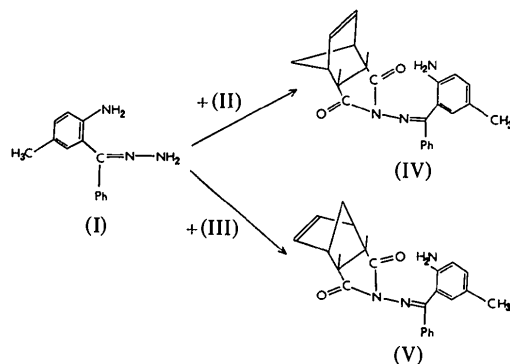
Experimental. Both compounds (IV) and (V) (melting points 526 and 516 K from toluene) gave satisfactory elemental analyses. Their X-ray structures are in full agreement with IR, PMR and mass spectra.

Pale yellow plate-like crystals 0·6 × 0·5 × 1·3 mm (IV) and 0·7 × 0·4 × 1·5 mm (V), three-circle single-crystal DAR-UMB diffractometer, graphite-mono-chromated Cu $K\alpha$ radiation, combined ω and $\theta/2\theta$ scan mode, scan speed 8° min^{-1}. Three reflections were used for the lattice-parameters determination; 3564 (IV) and 3634 (V) independent reflections were collected in the range $2 \le \theta \le 57°$ (h 0→13; k −13→13; l 0→15) for (IV), (h 0→13; k −14→14; l 0→16) for (V); 2801 (IV) and 2804 (V) reflections with $I \ge 3\sigma(I)$ were used for calculations. 16 standard reflections (one in each layer)

were monitored during data collection without detecting significant decay of intensity. Lp corrections. No absorption or extinction corrections. Direct method; H atoms located from difference Fourier maps.

Full-matrix least-squares anisotropic refinement on F for non-H atoms and isotropic refinement for H atoms using the weighting scheme $w = [\sigma(F)^2 + 0.01|F|^2]^{-1}$ led to $R = 0.056$ ($wR = 0.064$) (IV) and $R = 0.055$ ($wR = 0.066$) (V). Max. $\Delta/\sigma = 0.233$ (IV) and 0.412 (V). $\Delta\rho$ on the final difference Fourier synthesis 0.13 (IV) and 0.14 (V) e Å^{-3}. The atomic scattering parameters with f' and f'' were taken from Cromer & Waber (1974). The calculations were carried out on an

ES computer with the *YANX* programs (Gerr, Yanovsky & Struchkov, 1983).

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($\times 10^4$)

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

	x	y	z	$U_{eq}(\text{Å}^2)$
Compound (IV)				
N(1)	7478 (1)	5527 (1)	3245 (1)	534 (9)
N(2)	7791 (1)	5068 (1)	895 (1)	458 (7)
N(3)	8214 (1)	5404 (1)	−238 (1)	417 (7)
O(1)	7562 (1)	7108 (1)	−447 (1)	592 (8)
O(2)	9142 (1)	3960 (1)	−306 (1)	695 (10)
C(1)	6732 (1)	4791 (1)	3055 (1)	411 (8)
C(2)	6508 (1)	4215 (1)	1905 (1)	369 (8)
C(3)	5734 (1)	3432 (1)	1830 (1)	404 (8)
C(4)	5175 (1)	3197 (2)	2816 (2)	470 (9)
C(5)	5410 (1)	3783 (2)	3931 (2)	529 (10)
C(6)	6143 (1)	4552 (2)	4048 (1)	494 (9)
C(7)	7039 (1)	4452 (1)	793 (1)	364 (8)
C(8)	4349 (1)	2349 (2)	2700 (2)	648 (12)
C(9)	8099 (1)	6488 (1)	−778 (1)	426 (8)
C(10)	8750 (1)	6707 (1)	−1813 (1)	427 (9)
C(11)	9285 (1)	5641 (1)	−1765 (1)	442 (9)
C(12)	8908 (1)	4867 (1)	−702 (1)	451 (9)
C(13)	9119 (1)	5054 (2)	−3070 (1)	555 (11)
C(14)	9555 (1)	5988 (2)	−3961 (2)	599 (11)
C(15)	9089 (1)	6888 (2)	−3998 (2)	620 (12)
C(16)	8332 (1)	6607 (2)	−3135 (2)	530 (10)
C(17)	8171 (1)	5237 (2)	−3280 (2)	601 (11)
C(18)	6703 (1)	3958 (1)	−429 (1)	357 (7)
C(19)	7009 (1)	2934 (1)	−896 (1)	472 (9)
C(20)	6722 (1)	2502 (2)	−2047 (2)	543 (10)
C(21)	6152 (1)	3080 (2)	−2728 (2)	521 (10)
C(22)	5846 (1)	4083 (2)	−2264 (2)	529 (10)
C(23)	6120 (1)	4532 (1)	−1109 (2)	452 (9)
Compound (V)				
N(1)	7434 (1)	5519 (1)	3189 (1)	541 (8)
N(2)	7746 (1)	5105 (1)	809 (1)	459 (8)
N(3)	8182 (1)	5391 (1)	−331 (1)	406 (7)
O(1)	7547 (1)	7105 (1)	−560 (1)	731 (10)
O(2)	9120 (1)	3927 (1)	−347 (1)	645 (9)
C(1)	6702 (1)	4771 (1)	3019 (1)	404 (8)
C(2)	6483 (1)	4217 (1)	1867 (1)	349 (7)
C(3)	5708 (1)	3444 (1)	1805 (1)	393 (8)
C(4)	5158 (1)	3195 (1)	2804 (2)	424 (8)
C(5)	5392 (1)	3745 (2)	3935 (2)	507 (10)
C(6)	6130 (1)	4511 (2)	4038 (1)	498 (9)
C(7)	7011 (1)	4451 (1)	731 (1)	353 (8)
C(8)	4334 (1)	2375 (2)	2708 (2)	596 (11)
C(9)	8097 (1)	6455 (1)	−875 (1)	448 (9)
C(10)	8794 (1)	6637 (1)	−1871 (1)	459 (9)
C(11)	9304 (1)	5546 (2)	−1830 (2)	480 (10)
C(12)	8896 (1)	4822 (2)	−773 (2)	446 (9)
C(13)	9161 (1)	5038 (2)	−3181 (2)	586 (11)
C(14)	8175 (2)	4705 (2)	−3324 (2)	555 (11)
C(15)	7764 (1)	5643 (3)	−3357 (2)	679 (13)
C(16)	8439 (1)	6651 (2)	−3244 (2)	700 (13)
C(17)	9229 (1)	6187 (2)	−3918 (2)	591 (11)
C(18)	6678 (1)	3925 (1)	−472 (1)	338 (7)
C(19)	6987 (1)	2891 (2)	−886 (2)	445 (9)
C(20)	6684 (1)	2408 (2)	−2009 (2)	522 (10)
C(21)	6084 (1)	2961 (2)	−2726 (2)	501 (10)
C(22)	5765 (1)	3976 (2)	−2297 (2)	507 (10)
C(23)	6061 (1)	4460 (1)	−1179 (2)	436 (9)

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

	Compound (IV)	Compound (V)
C(1)—C(2)	1.425 (2)	1.418 (2)
C(2)—C(3)	1.409 (2)	1.415 (2)
C(3)—C(4)	1.382 (2)	1.371 (2)
C(4)—C(5)	1.401 (2)	1.401 (2)
C(5)—C(6)	1.354 (3)	1.370 (3)
C(6)—C(1)	1.418 (2)	1.409 (2)
C(1)—N(1)	1.361 (2)	1.362 (2)
C(4)—C(8)	1.514 (3)	1.505 (2)
C(2)—C(7)	1.466 (2)	1.468 (2)
C(7)—C(18)	1.502 (2)	1.495 (2)
C(18)—C(19)	1.388 (2)	1.389 (2)
C(19)—C(20)	1.390 (2)	1.389 (2)
C(20)—C(21)	1.373 (3)	1.381 (3)
C(21)—C(22)	1.367 (3)	1.381 (3)
C(22)—C(23)	1.394 (2)	1.382 (2)
C(23)—C(18)	1.385 (2)	1.383 (2)
C(7)—N(2)	1.294 (2)	1.293 (2)
N(2)—N(3)	1.421 (2)	1.414 (2)
N(3)—C(9)	1.378 (2)	1.376 (2)
C(9)—O(1)	1.203 (2)	1.210 (3)
C(9)—C(10)	1.511 (2)	1.501 (2)
C(10)—C(11)	1.536 (3)	1.528 (3)
C(11)—C(12)	1.516 (2)	1.510 (2)
C(12)—O(2)	1.198 (2)	1.203 (2)
C(12)—N(3)	1.392 (2)	1.388 (2)
C(11)—C(13)	1.565 (2)	1.571 (3)
C(13)—C(14)	1.523 (3)	1.513 (3)
C(14)—C(15)	1.311 (3)	1.291 (4)
C(15)—C(16)	1.508 (3)	1.490 (3)
C(16)—C(10)	1.569 (2)	1.567 (2)
C(16)—C(17)	1.534 (3)	1.525 (3)
C(17)—C(13)	1.533 (3)	1.542 (3)
C(1)—C(2)—C(3)	118.6 (1)	118.5 (1)
C(2)—C(3)—C(4)	123.3 (1)	123.4 (1)
C(3)—C(4)—C(5)	116.7 (2)	117.0 (1)
C(4)—C(5)—C(6)	122.2 (2)	121.7 (2)
C(5)—C(6)—C(1)	122.0 (1)	121.8 (2)
C(6)—C(1)—C(2)	117.1 (1)	117.5 (1)
N(1)—C(1)—C(2)	123.6 (1)	123.5 (1)
N(1)—C(1)—C(6)	119.3 (1)	119.0 (1)
C(3)—C(4)—C(8)	121.8 (2)	122.3 (2)
C(5)—C(4)—C(8)	121.5 (2)	120.7 (2)
C(1)—C(2)—C(7)	122.0 (1)	122.4 (1)
C(3)—C(2)—C(7)	119.4 (1)	119.1 (1)
C(2)—C(7)—N(2)	119.0 (1)	118.7 (1)
N(2)—C(7)—C(18)	121.8 (1)	122.5 (1)
C(2)—C(7)—C(18)	119.3 (1)	118.8 (1)
C(7)—C(18)—C(19)	119.0 (1)	120.1 (1)
C(7)—C(18)—C(23)	121.0 (1)	120.4 (1)
C(18)—C(19)—C(20)	119.1 (2)	120.1 (2)
C(19)—C(20)—C(21)	121.0 (2)	120.2 (2)
C(20)—C(21)—C(22)	119.9 (2)	119.5 (2)
C(21)—C(22)—C(23)	120.2 (2)	120.7 (2)
C(22)—C(23)—C(18)	119.9 (2)	120.1 (2)
C(23)—C(18)—C(19)	119.9 (1)	119.5 (1)
C(7)—N(2)—N(3)	115.6 (1)	116.2 (1)
N(2)—N(3)—C(9)	119.6 (1)	120.1 (1)
N(2)—N(3)—C(9)	123.8 (1)	123.2 (1)
N(3)—C(9)—O(1)	123.7 (2)	123.6 (2)
N(3)—C(12)—O(2)	124.6 (1)	124.0 (2)
O(1)—C(9)—C(10)	128.8 (2)	128.1 (2)
O(2)—C(12)—C(11)	128.3 (2)	129.2 (2)
C(9)—C(10)—C(11)	105.3 (1)	104.8 (1)
C(10)—C(11)—C(12)	105.1 (1)	105.7 (1)
C(11)—C(12)—N(3)	107.1 (1)	106.9 (1)
C(12)—N(3)—C(9)	114.6 (1)	114.2 (1)
N(3)—C(9)—C(10)	107.6 (1)	108.3 (1)
C(10)—C(11)—C(12)	102.6 (1)	102.6 (1)
C(11)—C(13)—C(14)	104.0 (1)	106.9 (2)
C(13)—C(14)—C(15)	107.8 (2)	108.4 (2)
C(14)—C(15)—C(16)	108.1 (2)	108.2 (2)
C(15)—C(16)—C(17)	100.3 (2)	100.9 (2)
C(16)—C(17)—C(13)	94.1 (2)	93.4 (2)
C(17)—C(13)—C(14)	100.0 (2)	99.5 (2)
C(12)—C(11)—C(13)	114.1 (1)	116.5 (2)
C(11)—C(13)—C(17)	101.1 (1)	98.8 (2)
C(11)—C(10)—C(16)	103.5 (1)	103.3 (1)
C(10)—C(16)—C(15)	103.9 (2)	106.3 (2)
C(10)—C(16)—C(17)	100.5 (1)	99.5 (2)
C(9)—C(10)—C(16)	113.4 (1)	115.7 (1)

Discussion. The final atomic positions of non-H atoms are presented in Table 1.* Figs. 1 and 2 illustrate the molecular structures of (IV) and (V) with atomic labelling. Bond distances and angles are given in Table 2. Table 3 presents selected dihedral angles of the structures. Molecular structures (IV) and (V) are similar; hence their unit-cell parameters are similar and the crystals are almost isostructural. The difference between (IV) and (V) involves the different conformation of the dicarboximidonorbornene fragments: in (IV) the combination of the five-membered dicarboximido fragment and the six-membered norbornene rings has a chair conformation (*exo* configuration), while in (V) it has a boat form (*endo* configuration). Different intermolecular contacts in the unit cell lead to some differences in conformational parameters. Other differences in the molecular geometry are insignificant. The molecules of the *exo* and *endo* conformers were

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44126 (37 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
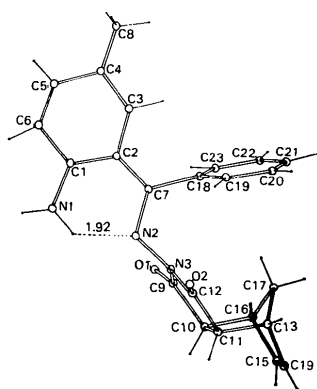

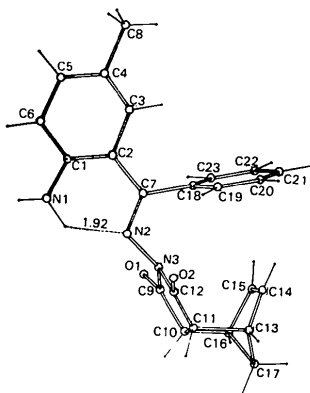Fig. 1. Projection of the *exo*-isomer molecule on the C(1)—C(6) benzene-ring plane.

Fig. 2. Projection of the *endo*-isomer molecule on the C(1)—C(6) benzene-ring plane.

Table 3. *Selected dihedral angles* (°) (*e.s.d.'s ca* 0·2°)

	Compound (IV)	Compound (V)
C(1)—C(2)—C(7)—N(2)	−9·8	−6·4
C(2)—C(7)—N(2)—N(3)	171·5	174·1
C(2)—C(7)—C(18)—C(19)	101·5	96·0
C(7)—N(2)—N(3)—C(9)	−91·3	−100·3
C(12)—C(11)—C(13)—C(14)	179·8	−50·6
C(9)—C(10)—C(16)—C(15)	−178·5	46·0
C(12)—C(11)—C(13)—C(17)	−76·8	−153·3
C(9)—C(10)—C(16)—C(17)	78·0	150·4
C(10)—C(16)—C(17)—C(13)	56·8	−59·4
C(11)—C(13)—C(17)—C(16)	−57·5	60·3
C(9)—C(10)—C(11)—C(12)	−0·1	2·4
C(9)—C(10)—C(11)—C(13)	−119·7	−120·1
C(16)—C(10)—C(11)—C(12)	119·2	124·0
N(3)—C(12)—C(11)—C(13)	109·2	108·6
C(9)—N(3)—C(12)—C(11)	4·4	5·3
C(10)—C(9)—N(3)—C(12)	−4·5	−3·8
C(11)—C(13)—C(14)—C(15)	71·7	−69·4
C(17)—C(13)—C(14)—C(15)	−32·5	32·9
C(13)—C(14)—C(15)—C(16)	−0·5	−0·2
C(14)—C(15)—C(16)—C(10)	−70·3	70·2
C(14)—C(15)—C(16)—C(17)	33·3	−33·2

brought to coincidence using a least-squares procedure with the exclusion of atoms C(13)—C(17) of the five-membered ring which has a different orientation in (IV) and (V); the mean atomic deviation was $S = (\sum_i \Delta r_i^2 / N)^{1/2} = 0·09$ Å, where Δr_i is the distance between the corresponding atoms in both moelcules. The small S value emphasizes the similarity of both configurational and conformational parameters of the molecules (Tables 2, 3). Indeed, all the bond distances are identical within experimental errors. For all bonds the difference in distances does not exceed 0·020 Å, and the average standard deviation is 0·011 Å. The most remarkable differences in bond angles with standard deviations of 0·8° occur in the norbornene fragment (where they reach 3·0°), which is caused by the conformational change of the latter. Besides the conformational changes of the norbornene fragment there are differences in the torsion angles and rotation angles of the phenyl ring between two isomers. The differences in torsion angles along the C(1)—C(2)—C(7)—N(2)—N(3)—C(9)—C(10) chain range from 2·6 to 9·0° (Table 3) but dihedral angles between phenyl rings differ by 3·7° and are equal to 98·5 and 94·8° for *exo* and *endo* conformers respectively. Such differences in *exo* and *endo* isomer conformations cannot be considered significant and are explained by the different packing conditions. Both isomers possess C(2),N(3)-*trans* configurations [the torsion angle around the N(2)=C(7) bond being 171·5° (IV) and 174·1° (V)] and a C(1),N(2)-*cis* conformation around the C(2)—C(7) bond [the corresponding torsion angle being −9·8° in (IV) and −6·4° in (V)]. The latter conformation is stabilized by the strong intramolecular H bond N(1)—H···N(2) [for the *exo* isomer: N(1)···N(2) = 2·648, N(1)—H = 0·94, N(2)···H = 1·92 Å, N(1)—H—N(2) = 133°; for the *endo* isomer: N(1)···N(2) = 2·643, N(1)—H = 0·95, N(2)···H = 1·92 Å, N(1)—H—N(2) = 131°]. Such intramolecular H bonds are typical of *trans* isomers of hydrazones (Dvorkin,

$C_{23}H_{21}N_3O_2$

Simonov, Gifeysman, Malinovsky, Andronati & Yavorsky, 1985). The second hydrogen atom of the NH_2 group is involved in intermolecular hydrogen bonding, which links the molecules in spirals around the 2_1 axis and whose parameters are: $N(1)\cdots O = 3\cdot011$, $N(1)-H = 0\cdot90$, $O(1)\cdots H = 2\cdot27$ Å, $N(1)-H-O(1) = 139°$ for the *exo* isomer and $N(1)\cdots O(1) = 3\cdot056$, $N(1)-H = 0\cdot91$, $O(1)\cdots H = 2\cdot26$ Å, $N(1)-H-O(1) = 146°$ for the *endo* isomer. The five-membered $C(9)-C(12)$, $N(3)$ ring is essentially planar (atomic deviations from the mean plane not exceeding $0\cdot03$ Å). The O atoms are displaced by $0\cdot067$ (*exo* isomer) and $0\cdot112$ Å (*endo* isomer) from this plane, both in the same direction. In the norbornene moiety the angles between planes $C(10)$, $C(11)$, $C(13)$, $C(16)$ and $C(13)$, $C(17)$, $C(16)$, *i.e.* the flapping angles of the five-membered envelope rings, are $61\cdot5$ and $59\cdot0°$ for the *exo* and *endo* isomers respectively, while the bending angles between planes $C(10)$, $C(11)$, $C(13)$, $C(16)$ and $C(13)-C(16)$ in the six-membered rings are $70\cdot4$ and $112\cdot7°$ for the *exo* and *endo* isomers respectively. The volumes occupied by the $C(14)H$, $C(15)H$ and $C(17)H_2$

groups are rather close so that the molecular packing should change only insignificantly if the conformation of the norbornene fragment is changed, which is indicated by the great similarity in both crystal and molecular structures.

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Structure of N-(2-Chloroethyl)-2-furamide

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Abstract. $C_7H_8ClNO_2$, $M_r = 173\cdot60$, monoclinic, $P2_1/c$, $a = 9\cdot348$ (3), $b = 9\cdot887$ (3), $c = 9\cdot693$ (5) Å, $\beta = 116\cdot35$ (4)°, $V = 802\cdot8$ (6) Å^3, $Z = 4$, $D_x = 1\cdot436$ g cm^{-3}, λ(Mo $K\alpha$) = $0\cdot7107$ Å, $\mu = 4\cdot21$ cm^{-1}, $F(000) = 360$, $T = 293$ K, final $R = 0\cdot045$ for 914 observed reflections. The non-H atoms of the molecule, except the terminal C atom and the Cl atom attached to it, deviate within $\pm0\cdot049$ (5) Å from their mean plane. The exocyclic bond angles at the C(2) and C(5) atoms of the furan ring show marked differences: $C-C(2)-C = 131\cdot7$ (4), $C-C(2)-O = 119\cdot0$ (4) and $H-C(5)-C = 130$ (3), $H-C(5)-O = 119$ (3)°, respectively.

These differences, common for furan compounds in the comparable range, may be due to possible rehybridization effects at the C(2) and C(5) atoms. The C=O and C(sp^2)—N bond lengths are $1\cdot236$ (4) and $1\cdot337$ (6) Å, respectively. The molecules are connected by N—H···O(=C) hydrogen bonds of $2\cdot872$ (5) Å in chains along the c axis.

Introduction. Compounds with one or more N-(2-chloroethyl) moieties show many pharmacological activities. They are cytotoxic (Bodenstein & Goldin, 1948), mutagenic (Auerbach & Moser, 1950), immuno-