0·007 Å (1·4σ) shorter and C(1)–C(11) and C(11)–C(14′) are longer by 0·020 Å (3·3σ) and 0·029 Å (4·8σ), respectively, in the present compound. The bond lengths in the present compound agree with those in naphtho[1,8:4,5]dicyclopentene (Simmons & Lingafelter, 1961) within the precision of the earlier work.

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Structure of Halopemide, an Antipsychotic Benzamide Derivative

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Abstract. $C_{21}H_{22}ClFN_4O_2$; *N*-{2-[4-(5-chloro-2-oxo-1-benzimidazolinyl)piperidino]ethyl}-*p*-fluorobenzamide; triclinic, $P\bar{1}$; a = 14·322 (5), b = 15·057 (5), c = 10·271 (5) Å, α = 103·94 (5), β = 110·86 (5), γ = 92·67 (5)°; D_m = 1·38 (2), D_c = 1·39 Mg m^{-3}, Z = 4, T = 294 K. The molecules form dimers linked through the endocyclic amide groups (imidazolinone group); moreover, each molecule is hydrogen bonded to two neighbours through the exocyclic amide group (benzamide group).

Introduction. Halopemide is an anti-autistic benzamide derivative related to the class of butyrophenones. The space group was determined from photographs. The final cell dimensions and intensities were measured on a Nonius CAD-4 four-circle computer-controlled diffractometer. The instrumental settings are given in Table 1. No corrections were made for absorption.

The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971). Three fragments containing 48 atoms were found in the most probable E map. Three successive Fourier maps revealed the two molecules of the asymmetric unit, H atoms excepted. Full-matrix least-squares refinement was performed with XRAY 72 (Stewart, Kruger, Ammon, Dickinson & Hall, 1972) minimizing $\sum w(F_o - F_c)^2$; the weight w

Table 1. *Instrumental settings for the data collection*

Crystal size: 0·5 × 0·4 × 0·2 mm
Source: Cu $K\bar{\alpha}$; λ = 1·54178 Å
Graphite monochromator
$2 \le \theta \le 65°$
$\Delta 2\theta = 0·75 + 0·14 \text{ tg } \theta$ (°)
Aperture = 2·5 + 0·5 tg θ (mm)
Confidence level: 2·5σ, where $\sigma^2 = S + B + (0·03S)^2$, S being the scan and B the background count
Total number of independent reflexions: 5361
Total observed: 2535

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0567-7408/80/040965-03$01.00

Table 2. *Final coordinates* ($\times 10^4$, *for* $z \times 10^3$), *with e.s.d.'s in parentheses, and* U_{eq} *values* (Å$^2 \times 10^4$)

$$U_{eq} = (U_{11} . U_{22} . U_{33})^{1/3}.$$

	x	y	z	U_{eq}		x	y	z	U_{eq}
Cl(1)	5418 (3)	4159 (3)	217 (1)	694	Cl(101)	19634 (3)	5934 (3)	293 (1)	817
C(2)	6352 (9)	4003 (9)	149 (1)	493	C(102)	18645 (9)	6030 (9)	354 (1)	527
C(3)	6399 (9)	4478 (9)	51 (1)	437	C(103)	18586 (9)	5549 (9)	447 (1)	533
C(4)	7211 (9)	4367 (8)	6 (1)	413	C(104)	17841 (8)	5703 (8)	497 (1)	342
N(5)	7440 (7)	4708 (6)	−93 (1)	373	N(105)	17580 (7)	5306 (7)	592 (1)	510
C(6)	8234 (9)	4356 (9)	−111 (1)	406	C(106)	16755 (8)	5641 (9)	610 (1)	393
O(7)	8623 (6)	4501 (6)	−195 (1)	675	O(107)	16369 (6)	5523 (7)	695 (1)	651
N(8)	8541 (7)	3811 (7)	−19 (1)	436	N(108)	16452 (7)	6214 (7)	522 (1)	464
C(9)	7875 (8)	3790 (7)	51 (1)	418	C(109)	17121 (9)	6274 (9)	452 (1)	496
C(10)	7839 (9)	3310 (9)	150 (1)	722	C(110)	17195 (9)	6729 (9)	357 (2)	569
C(11)	7038 (9)	3428 (9)	196 (1)	725	C(111)	17967 (9)	6596 (9)	305 (2)	644
C(12)	9416 (8)	3347 (8)	−16 (1)	338	C(112)	15610 (9)	6725 (9)	517 (1)	539
C(13)	9095 (9)	2354 (9)	−102 (1)	534	C(113)	14862 (9)	6622 (8)	367 (2)	498
C(14)	9990 (9)	1864 (9)	−110 (1)	568	C(114)	13995 (9)	7130 (9)	380 (2)	647
N(15)	10711 (7)	1969 (7)	38 (1)	434	N(115)	14314 (7)	8092 (7)	468 (1)	346
C(16)	11024 (9)	2909 (8)	123 (1)	370	C(116)	14987 (9)	8106 (9)	607 (1)	526
C(17)	10120 (9)	3367 (9)	134 (1)	383	C(117)	15903 (9)	7666 (9)	608 (1)	518
C(18)	11583 (9)	1484 (9)	34 (1)	500	C(118)	13419 (9)	8484 (9)	469 (1)	526
C(19)	11261 (9)	438 (9)	−32 (1)	526	C(119)	13639 (9)	9486 (9)	540 (1)	554
N(20)	12160 (9)	20 (8)	−29 (1)	609	N(120)	12772 (8)	9962 (8)	497 (1)	552
C(21)	12700 (9)	−360 (8)	72 (1)	834	C(121)	12182 (8)	10245 (7)	574 (1)	548
O(22)	12543 (9)	−134 (7)	199 (1)	770	O(122)	12406 (8)	10121 (8)	702 (1)	799
C(23)	13607 (9)	−730 (9)	70 (2)	779	C(123)	11379 (9)	10787 (9)	511 (2)	552
C(24)	14145 (9)	−1050 (9)	177 (2)	925	C(124)	10770 (9)	11008 (9)	585 (2)	799
C(25)	14905 (9)	−1492 (9)	177 (2)	956	C(125)	9972 (9)	11436 (9)	529 (2)	726
C(26)	15189 (9)	−1610 (9)	72 (2)	758	C(126)	9806 (9)	11618 (9)	406 (2)	583
F(27)	15994 (9)	−2027 (9)	76 (2)	1400	F(127)	9008 (8)	12054 (7)	357 (1)	1064
C(28)	14721 (9)	−1273 (9)	−42 (2)	1509	C(128)	10373 (9)	11375 (9)	324 (2)	708
C(29)	13904 (9)	−782 (9)	−40 (2)	1125	C(129)	11242 (9)	10934 (9)	384 (2)	609
					H(20)	12555 (4)	0 (4)	−157 (1)	
					H(120)	12467 (5)	10211 (3)	357 (1)	

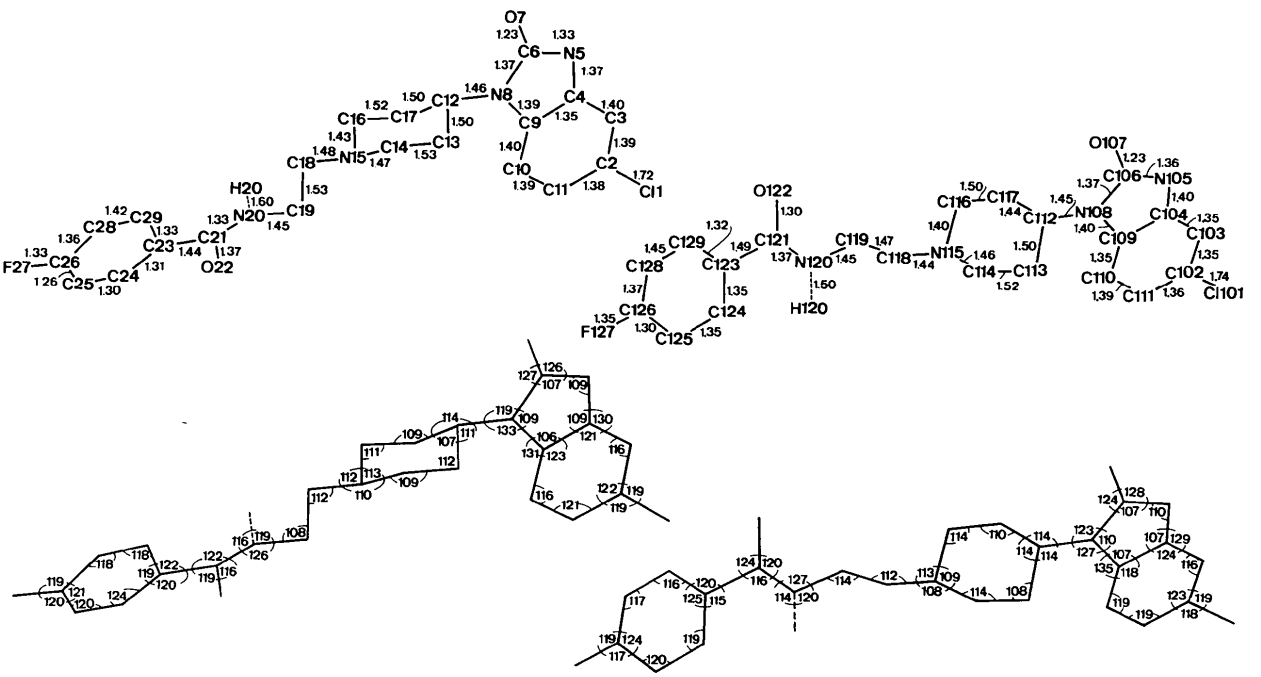

Fig. 1. Bond lengths (Å) and angles (°). The e.s.d.'s for distances and angles involving non-hydrogen atoms are in the ranges 0·01–0·03 Å and 1–2° respectively.

is given by: $w = 1/(AF_o + BF_o^2)$, where $A = 2F_o^{min}$ and $B = 2/F_o^{max}$ (Cruickshank, 1961).

All H atoms were located on a difference synthesis. With anisotropic temperature factors for all non-H atoms and isotropic for H, the final R was 0·09. The scattering factors were those of Cromer & Mann (1968) except for H (Stewart, Davidson & Simpson, 1965). The final coordinates are given in Table 2. Fig. 1 gives bond lengths and angles and the atom numbering. H(20) and H(120) are included in this table and figure.*

Discussion. Halopemide is structurally related to known potent neuroleptics. The piperidine adopts the usual chair form with the benzimidazolinone group in the equatorial position. The angle between the least-squares mean planes of the piperidine ring and the benzimidazolinone group is 78°. The presence of an aromatic group nearly perpendicular to the mean plane of the piperidine ring seems to be a requirement for strong antipsychotic activity. In benperidol (Declercq, Germain & Koch, 1973), clopimozide (Van Opdenbosch, Evrard, Durant & Koch, 1977) and 1-{1-[3-(2-trifluoromethyl-10-phenothiazinyl)propyl]-4-piperidinyl}-2-benzimidazolinone, a structurally similar phenothiazine derivative (Van Opdenbosch, Durant, Chawdhury & Koch, 1977), this conformation appears to be rigidly fixed.

The crystal conformations of the two molecules of halopemide can be described in terms of torsion angles which are summarized in Table 3. The two conformations are similar except for the value of the dihedral angle [C(19)–N(20)] between the benzamide group and the side chain.

The molecules form dimers similar to those found in clopimozide and the phenothiazine derivative. The dimerization is due to the imidazolinone groups which are hydrogen bonded: N(5)···O(107)($x-1$, y, $z-1$) 2·77, O(7)···N(105)($x-1$, y, $z-1$) 2·76 Å. Moreover, each molecule is hydrogen bonded to two neighbours: N(20)···O(122)(x, $y-1$, $z-1$) 2·95, O(22)···N(120)(x, $y-1$, z) 2·93 Å (e.s.d.'s < 0·03 Å). H(20) and H(120) are equally shared between N(20) and O(122), N(120) and O(22) respectively, explaining the unusual length of the intramolecular carbonyl distances.

Stereoscopic views of the packing and the molecules are shown in Figs. 2 and 3.

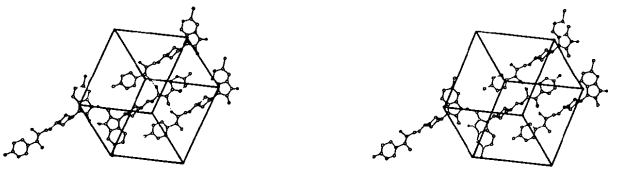

Fig. 2. Stereoscopic view of the crystal packing. For clarity, solid circles mark H(20) and H(120).

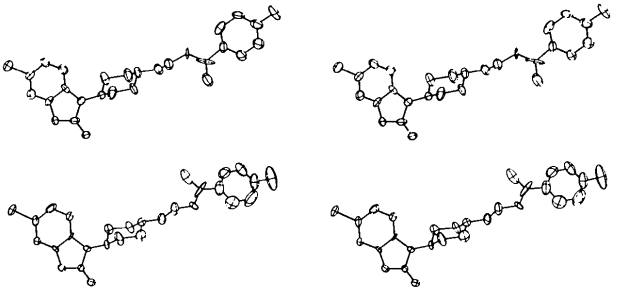

Fig. 3. Stereoscopic views of the molecules with 50% probability thermal ellipsoids.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34970 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 3. *Torsion angles* (°) *of the two molecules*

The convention used to define the torsion angle $\tau ABCD$ corresponds to a clockwise rotation of atom D into A viewed along the B–C axis (from B to C). Atomic coordinates of the second molecule have been inverted. E.s.d.'s ~3°.

C(6)–N(8)–C(12)–C(13)	−101	C(106)–N(108)–C(112)–C(117)	−96
C(6)–N(8)–C(12)–C(17)	138	C(106)–N(108)–C(112)–C(113)	130
C(14)–N(15)–C(18)–C(19)	−64	C(114)–N(115)–C(118)–C(119)	173
C(16)–N(15)–C(18)–C(19)	169	C(116)–N(115)–C(118)–C(119)	−67
N(15)–C(18)–C(19)–N(20)	−179	N(115)–C(118)–C(119)–N(120)	−158
C(18)–C(19)–N(20)–C(21)	97	C(118)–C(119)–N(120)–C(121)	−101
C(19)–N(20)–C(21)–C(23)	−178	C(119)–N(120)–C(121)–C(123)	−175
N(20)–C(21)–C(23)–C(24)	176	N(120)–C(121)–C(123)–C(124)	−176

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