layers are of a van der Waals type involving hydrophobic *tert*-butyl groups. The crystal cleavage perpendicular to the *a* axis is ascribed to this double-layered structure. In ten compounds having a bicyclooctane framework and hydroxyl groups found in a search of the Cambridge Structural Database (Allen, Kennard & Taylor, 1983) no such cleaved double-layered structure has been observed.

This work was supported in part by a Grant-in-Aid for Scientific Research on a Priority Area (No. 01628003) from the Japanese Ministry of Education, Science and Culture.

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Acta Cryst. (1992). C**48**, 1068–1071

Structure of an Anti-Arrhythmic and Hypotensive Agent: 1-{3-[4-(3-Chlorophenyl)-1-piperazinyl]-2-hydroxypropyl}pyrrolidin-2-one

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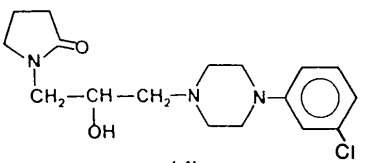
(*Received* 3 *June* 1991; *accepted* 1 *November* 1991)

Abstract. $C_{17}H_{24}ClN_3O_2$, $M_r = 337.85$, monoclinic, $P2_1/c$ (C_{2h}^5), $a = 15.492$ (2), $b = 6.592$ (1), $c = 17.193$ (2) Å, $\beta = 99.96$ (1)°, $V = 1729.3$ (4) Å^3, $Z = 4$, $D_m = 1.29$ (1), $D_x = 1.298$ (1) Mg m^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 0.23$ mm^{-1}, $F(000) = 720$, $T = 295$ K, $R = 0.0478$ for 1899 unique observed reflections [$F_o \geq 2\sigma(F_o)$]. The geometry of the amino-alcohol chain of the molecule, believed to be a pharmacophore, is antiperiplanar with an O(7)—C(7)—C(8)—N(9) torsion angle of −171.7 (2)° and an O(7)···N(9) distance of 3.742 (2) Å. It is associated with a relatively strong intermolecular hydrogen bond O(7)—H(O7)···O(2) translated by **b**, with O(7)···O(2) = 2.720 (3) Å. The compound exhibits anti-arrhythmic and hypotensive activity, as has been shown by pharmacological tests.

Introduction. Following the structure determination of 1-[2-hydroxy-3-(4-phenyl-1-piperazinyl)propyl]-pyrrolidin-2-one, refered to hereafter as (*B*) (Stadnicka, Ciechanowicz-Rutkowska & Malawska, 1991), we undertook the analogous study of its chloro derivative, 1-{3-[4-(3-chlorophenyl)-1-piperazinyl]-2-hydroxypropyl}pyrrolidin-2-one, (*A*).



(*A*)

The compound was synthesized and studied by Malawska, Gorczyca, Cebo & Krupińska (1988). It has anti-arrhythmic and hypotensive activity, weaker, however, than propranolol and quinidine but comparable to that of compound (*B*) (Malawska, Gorczyca, Filipek, Cros, Liutkus & Serrano, 1990).

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Experimental. Small colourless poor-quality crystals were obtained from a mixture of *n*-hexane and ethyl acetate. The crystal structure was successfully solved by direct methods (*MULTAN*11/82; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) in space group $P2_1/c$. Experimental data and details of the structure refinement are summarized in Table 1. The final atomic coordinates and thermal parameters are given in Table 2.* Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 149–150). Programs used include *SDP-Plus* (Frenz, 1983), *PARST* (Nardelli, 1983) and *ORTEP*II (Johnson, 1971).

Discussion. The molecular structure of compound (*A*), shown in Fig. 1, exhibits an antiperiplanar conformation for the N(9)—C(8)—C(7)—O(7) chain, similar to that of molecule (I) of compound (*B*) [hereafter called (*B*I)], and different from the synclinal conformation of molecule (II) of compound (*B*). This conformation might be imposed by stretching forces owing to the intermolecular hydrogen bonding.

Bond lengths, angles and selected torsion angles are given in Table 3.

The quantitative description of pyrrolidine and piperazine rings is given in terms of parameters defined by Nardelli (1983). The pyrrolidine five-membered ring has an envelope conformation with ring-puckering coordinates $q_2 = 0.092\ (3)$ Å and $\varphi_2 = -68\ (2)°$. A pseudo-mirror plane through C(4) was detected with a symmetry parameter [as defined by Nardelli (1983)] of 0.005 (1). The C—O bond length of 1.229 (3) Å is slightly longer than a usual carbonyl bond of 1.208 (7) Å (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987), because O(2) acts as an acceptor in an intermolecular hydrogen bond. The configuration at the pyrrolidine N atom is planar and its lone pair seems to be involved in the N(1)—C(2) bond, making it shorter than the neighbouring N—C bonds, as is similarly seen in molecule (*B*I).

The piperazine ring has the usual chair conformation with puckering coordinates $q_2 = 0.025\ (3)$, $q_3 = Q = 0.563\ (3)$ Å, $\varphi_2 = -60.3\ (1)$ and $\theta_2 = 2.6\ (3)°$. The asymmetry parameter for the pseudo-mirror plane through the N atoms is 0.016 (1). Again, similar to molecule (*B*I), the lone pair of N(14) interacts with the π system of the aromatic ring leading to shortening of N(14)—C(15) and a decrease in the

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54828 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AL0483]

Table 1. *Summary of data collection and structure refinement*

Crystal shape and size (mm)	Needle, *ca* 0.1 × 0.2 × 0.1
Method of measuring D_m	Flotation in aqueous KI
Diffractometer	Enraf–Nonius CAD-4 (graphite-monochromated Mo $K\alpha$ radiation)
Lattice-parameters measurement	
θ range (°), number of reflections	$5 \le \theta \le 17$, 25
Intensity measurement	
θ range (°)	$0 \le \theta \le 25$
Indices range	$0 \le h \le 18$, $0 \le k \le 7$, $-20 \le l \le 20$
Scan width (°) and mode	$1.0 + 0.35\tan\theta$, $\omega/2\theta$
Intensity control reflections	204, 402, 313 measured every hour
Changes in intensity (%)	< 3
Number of reflections measured (only unique reflections)	3032
Criterion for observed reflections	$I \ge 2\sigma(I)$
Number of observed reflections	1899
Corrections applied	Lorentz, polarization effects
Minimized function	$\sum w(F_o - F_c)^2$
Parameters refined	305
Non-H atoms	Positional and anisotropic thermal
H atoms*	Positional and isotropic thermal
Final value of secondary-extinction coefficient ($\times 10^8$)†	11 (4)
Weighting scheme	$w = 4I_o/[\sigma^2(I_o) + (PI_o)^2]$, where P (Peterson–Levy coefficient) was set to 0.02
R, wR, S	0.0478, 0.0434, 1.883
Average, max. Δ/σ	0.01, 0.17
Max., min. heights in final difference Fourier map (e Å^{-3})	0.25, −0.10

* Initial positional parameters of H atoms from the difference Fourier map.

† Defined by Larson (1967), equation (3).

Table 2. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$B_{eq} = [4/3][a^2B_{11} + b^2B_{22} + c^2B_{33} + ab(\cos\gamma)B_{12} + ac(\cos\beta)B_{13} + bc(\cos\alpha)B_{23}].$$

	x	y	z	B_{eq}
Cl(17)	0.97431 (6)	0.0681 (2)	0.39415 (6)	8.44 (3)
O(7)	0.3349 (1)	0.3958 (3)	−0.0148 (1)	4.65 (4)
O(2)	0.3244 (1)	−0.2291 (3)	0.0488 (1)	5.14 (5)
N(1)	0.2431 (1)	0.0580 (3)	0.0447 (1)	3.95 (5)
N(9)	0.5098 (1)	0.2324 (3)	0.1516 (1)	3.09 (4)
N(14)	0.6812 (1)	0.0551 (3)	0.2037 (1)	3.77 (5)
C(7)	0.3760 (2)	0.2620 (4)	0.0451 (1)	3.42 (6)
C(18)	0.9211 (2)	−0.2307 (6)	0.2914 (2)	6.90 (9)
C(6)	0.3106 (2)	0.1772 (4)	0.0925 (2)	4.10 (6)
C(2)	0.2574 (2)	−0.1327 (4)	0.0240 (2)	4.00 (6)
C(3)	0.1805 (2)	−0.2025 (5)	−0.0358 (2)	5.61 (8)
C(4)	0.1149 (2)	−0.0336 (5)	−0.0421 (2)	7.12 (9)
C(5)	0.1602 (2)	0.1432 (5)	0.0038 (2)	6.16 (8)
C(8)	0.4544 (2)	0.3625 (4)	0.0950 (1)	3.66 (6)
C(10)	0.5859 (2)	0.3529 (4)	0.1880 (1)	3.69 (6)
C(12)	0.6526 (2)	0.2319 (4)	0.2438 (2)	4.00 (6)
C(13)	0.6059 (2)	−0.0663 (4)	0.1677 (2)	4.08 (6)
C(11)	0.5423 (2)	0.0595 (4)	0.1116 (1)	3.80 (6)
C(15)	0.7594 (2)	−0.0409 (4)	0.2348 (1)	3.75 (6)
C(16)	0.8214 (2)	0.0464 (5)	0.2937 (2)	4.61 (7)
C(17)	0.9005 (2)	−0.0473 (5)	0.3198 (2)	5.47 (8)
C(19)	0.8603 (2)	−0.3217 (5)	0.2338 (2)	6.66 (9)
C(20)	0.7811 (2)	−0.2315 (5)	0.2073 (2)	5.21 (7)
H(O7)*	0.332 (2)	0.499 (4)	0.009 (1)	6.3 (4)

* Atom H(O7), which is involved in hydrogen bonding, was refined isotropically.

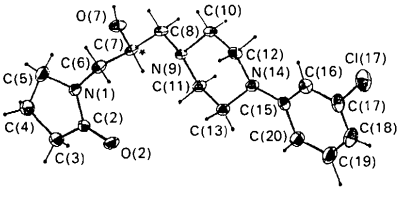

Fig. 1. *ORTEP*II (Johnson, 1971) drawing of the molecular structure of the title compound.

Table 3. *Bond lengths* (Å), *angles* (°) *and torsion angles* (°)

Cl(17)—C(17)	1.736 (3)	C(7)—C(8)	1.513 (4)
O(7)—C(7)	1.420 (3)	C(18)—C(17)	1.362 (5)
O(2)—C(2)	1.229 (3)	C(18)—C(19)	1.380 (4)
N(1)—C(6)	1.445 (3)	C(2)—C(3)	1.505 (4)
N(1)—C(2)	1.335 (3)	C(3)—C(4)	1.499 (4)
N(1)—C(5)	1.465 (3)	C(4)—C(5)	1.511 (4)
N(9)—C(8)	1.459 (3)	C(10)—C(12)	1.510 (4)
N(9)—C(10)	1.469 (3)	C(13)—C(11)	1.503 (4)
N(9)—C(11)	1.465 (3)	C(15)—C(16)	1.394 (4)
N(14)—C(12)	1.461 (4)	C(15)—C(20)	1.404 (4)
N(14)—C(13)	1.461 (3)	C(16)—C(17)	1.376 (4)
N(14)—C(15)	1.389 (3)	C(19)—C(20)	1.369 (4)
C(7)—C(6)	1.513 (4)	O(7)—H(O7)	0.80 (2)

C(2)—C(3)—C(4)	105.6 (2)	C(3)—C(4)—C(5)	106.7 (3)
C(2)—N(1)—C(5)	113.9 (2)	N(1)—C(5)—C(4)	104.1 (2)
C(6)—N(1)—C(5)	123.5 (2)	N(9)—C(8)—C(7)	116.3 (2)
C(6)—N(1)—C(2)	121.7 (2)	N(9)—C(10)—C(17)	113.3 (3)
C(10)—N(9)—C(11)	107.8 (2)	N(14)—C(12)—C(10)	110.6 (2)
C(8)—N(9)—C(11)	110.8 (2)	N(14)—C(13)—C(11)	110.9 (2)
C(8)—N(9)—C(10)	107.6 (2)	N(9)—C(11)—C(13)	111.6 (2)
C(13)—N(14)—C(15)	119.5 (2)	N(14)—C(15)—C(20)	121.4 (2)
C(12)—N(14)—C(15)	119.8 (2)	N(14)—C(15)—C(16)	122.5 (3)
C(12)—N(14)—C(13)	110.6 (2)	C(16)—C(15)—C(20)	116.0 (5)
O(7)—C(7)—C(8)	110.8 (2)	C(15)—C(16)—C(17)	120.1 (3)
O(7)—C(7)—C(6)	111.2 (2)	C(18)—C(17)—C(16)	122.1 (3)
C(6)—C(7)—C(8)	113.8 (2)	Cl(17)—C(17)—C(16)	118.6 (3)
C(17)—C(18)—C(19)	118.0 (3)	Cl(17)—C(17)—C(18)	119.2 (3)
N(1)—C(6)—C(7)	112.4 (2)	C(18)—C(19)—C(20)	120.7 (3)
O(2)—C(2)—N(1)	124.3 (3)	C(15)—C(20)—C(19)	122.0 (3)
N(1)—C(2)—C(3)	108.8 (2)	C(7)—O(7)—H(O7)	102 (1)
O(2)—C(2)—C(3)	126.9 (3)		

C(6)—N(1)—C(2)—O(2)	7.0 (4)	O(7)—C(7)—C(8)—N(9)	−171.7 (2)
C(2)—N(1)—C(5)—C(4)	6.4 (3)	C(6)—C(7)—C(8)—N(9)	62.2 (3)
C(5)—N(1)—C(6)—C(7)	−90.2 (3)	C(8)—C(7)—C(6)—N(1)	−171.9 (2)
C(2)—N(1)—C(6)—C(7)	78.7 (3)	C(19)—C(18)—C(17)—Cl(17)	178.3 (3)
C(5)—N(1)—C(2)—C(3)	−0.9 (3)	C(17)—C(18)—C(19)—C(20)	−1.2 (5)
C(10)—N(9)—C(11)—C(13)	57.5 (3)	C(19)—C(18)—C(17)—C(16)	0.9 (5)
C(11)—N(9)—C(8)—C(7)	57.0 (3)	N(1)—C(2)—C(3)—C(4)	−5.1 (3)
C(10)—N(9)—C(8)—C(7)	174.6 (2)	C(2)—C(3)—C(4)—C(5)	8.8 (3)
C(11)—N(9)—C(10)—C(12)	−56.2 (3)	C(3)—C(4)—C(5)—N(1)	−9.2 (3)
C(13)—N(14)—C(15)—C(16)	−155.6 (3)	N(9)—C(10)—C(12)—N(14)	55.7 (3)
C(12)—N(14)—C(15)—C(16)	−13.4 (4)	N(14)—C(13)—C(11)—N(9)	−59.4 (3)
C(13)—N(14)—C(15)—C(20)	25.5 (4)	C(16)—C(15)—C(20)—C(19)	−3.2 (4)
C(12)—N(14)—C(15)—C(20)	167.7 (3)	C(20)—C(15)—C(16)—C(17)	2.9 (4)
C(12)—N(14)—C(13)—C(11)	56.6 (3)	C(15)—C(16)—C(17)—C(18)	−1.9 (5)
C(13)—N(14)—C(12)—C(10)	−54.3 (3)	C(15)—C(16)—C(17)—Cl(17)	−179.2 (2)
O(7)—C(7)—C(6)—N(1)	62.2 (3)	C(18)—C(19)—C(20)—C(15)	2.5 (5)

C(16)—C(15)—C(20) bond angle. The phenyl ring is planar. The phenyl-ring plane is inclined to the mean piperazine plane at an angle of 5.6 (1)° [7.0 (1)° for (*BI*)] and to the mean pyrrolidine plane at 7.9 (1)° [30.7 (2)° for (*BI*)]. The angle between the piperazine and pyrrolidine mean planes is 2.8 (1)° [26.3 (2)° for (*BI*)]. The hydroxyl group acts as a donor in a relatively strong hydrogen bond to the pyrrolidine O atom of the molecule shifted along **b**: O(7)···O(2) = 2.720 (3), O(7)—H(O7) = 0.80 (2), H(O7)···O(2) = 1.93 (3) Å, and O(7)—H(O7)···O(2)(x, $y+1$, z) = 170 (2)°. The values of analogous parameters describing the hydrogen bond in (*BI*) are 2.712 (2), 0.85 (1), 1.86 (1) Å, and 173 (2)°, respectively. There are no other intermolecular contacts which are shorter than the sum of the appropriate van der Waals radii.

The packing of the molecules is shown in Fig. 2. As can be seen in the (010) projection, all molecules are oriented in such a way that their longest axis is approximately parallel to [201]. The molecules having the same configuration and bound by the hydrogen bond form columns along [010]. The absolute configuration of the molecules in the columns in direction [$\bar{1}$02] is *S*, *S*, *R*, *R*.

For the compounds of pharmacological importance the geometry of the pharmacophore is always the point of interest. It can be described by the parameters calculated by analogy to those evaluated for compound (*BI*) for the β-aminoethanol chain in its relation to the receptor-pocket model (Stadnicka, Ciechanowicz-Rutkowska & Malawska, 1991).

The comparison is given in Table 4, where n_N is the number of bonds between the basic N atom and the π ring, d_N is the distance between the basic N and the farthest point of the hydrophobic moiety, N···π is the distance of the basic N from the π-ring plane, X···π is the analogous distance for the so-called 'helpful' heteroatom X (Schwalbe & Scott, 1979), N···X is the distance of the basic N from the 'helpful' heteroatom, and N—C—C—X is the relevant torsion angle. It can be seen that the geometry of the studied molecule, in spite of the bulky Cl substituent, is the same (antiperiplanar) as that for (*BI*) in the crystal state. It is also striking that if we part with the widely accepted N^+—C—C—O pharmacophore and accept the N^+—C—C—N fragment of the fairly rigid piperazine ring as such, with the N(14) atom recognized as a 'helpful' heteroatom instead of atom O(7), only the phenyl ring interacting as a hydrophobic moiety lies at the right site with respect to the basic N atom. If the pyrrolidine ring would act as the hydrophobic moiety the hydroxyl O atom would have to play the part of a 'helpful' heteroatom with N(9) again being the basic N atom. However, the antiperiplanar conformation of such a pharmacophore is much less frequent among the anti-arrhythmics [see Table 5 in Stadnicka, Ciechanowicz-Rutkowska & Malawska (1991)]. We are aware that in living organisms when

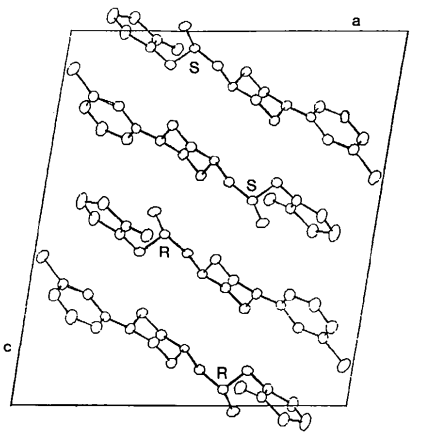

Fig. 2. Packing of the molecules shown in (010) projection.

Table 4. *Comparison of some geometrical parameters for non-substituted and chloro-substituted compounds (e.s.d.'s are about 0.002 Å for distances and 0.2° for angles)*

	$n_N d_N$	N···π (Å)	X	X···π (Å)	N···X (Å)	N—C—C—X (°)
Phenyl side			>N—			
This work	4 7.10	0.09		0.08	2.90	55.7
(*BI*)*	4 7.08	−0.25		0.12	2.89	−57.7
Pyrrolidine side			OH			
This work	6.42†	1.13		2.40	3.74	−171.7
(*BI*)*	6.17	0.31		−2.19	3.72	173.7

* Stadnicka, Ciechanowicz-Rutkowska & Malawska (1991).
† Distance of N atom from the midpoint between C(4) and C(3).

drugs interact with the receptor their molecules can be treated neither as free nor as restrained by exactly the same force field as in the crystal lattice. NMR studies are planned to determine the conformer population in solution.

This research was partly supported by the Polish Ministry of Education under Project No. RP.II.13.

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Acta Cryst. (1992). C**48**, 1071–1074

Structure of 1,3,5-Tribenzoylperhydro-1,3,5-triazine

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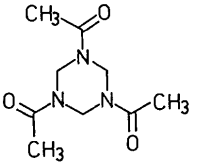
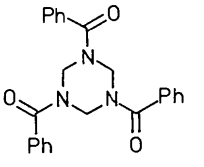
(*Received* 31 *July* 1991; *accepted* 29 *October* 1991)

Abstract. $C_{24}H_{21}N_3O_3$, $M_r = 399.45$, orthorhombic, $Pna2_1$, $a = 11.313$ (1), $b = 19.187$ (1), $c = 9.6363$ (9) Å, $V = 2091.6$ (3) Å^3, $Z = 4$, $D_x = 1.268$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 0.08$ mm^{-1}, $F(000) = 840$, $T = 298$ K, $R = 0.060$ for 1605 unique reflections. The molecular structure is asymmetric and the N atoms have approximate trigonal structures. The crystals show significant second-order harmonic generation and a short cut-off wavelength for absorption (298 nm).

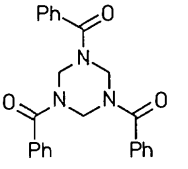
Introduction. While the molecular structures and intramolecular motions of 1,3,5-trialkyl- (or triaryl-) perhydro-1,3,5-triazines in the crystalline state as well as in the liquid phase have been extensively studied (Sim, 1987; Zangrando, Poggi, Giumanini & Verardo, 1987; Bouchemma, McCabe & Sim, 1988, 1990), those of 1,3,5-triacyl- (or triaroyl-) perhydro-1,3,5-triazines are much less well known. The crystal structure data of the latter have been found only for 1,3,5-triacetylperhydro-1,3,5-triazine (1) (Choi, Santoro & Marinkas, 1975) in the Cambridge Structural Database (1991).



(1)



(2*a*)



(2*b*)

Katritzky and his coworkers revealed that the title compound (2) exists as a mixture of the C_3 symme-

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