Kennard & Taylor, 1983) revealed only one X-ray structure of a tetra-substituted valerolactone in which the lactone was not bridged or fused to other rings (D-glucono-1,5-lactone; Hackert & Jacobson, 1971).

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Structure of 1-(2,6-Dimethylphenoxy)-2-propanamine Hydrochloride

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Abstract. $C_{11}H_{18}NO^+.Cl^-$, $M_r = 215.7$, triclinic, $P\bar{1}$, $a = 8.796$ (15), $b = 10.601$ (18), $c = 14.229$ (24) Å, $\alpha = 78.74$ (13), $\beta = 79.89$ (14), $\gamma = 68.69$ (12)°, $V = 1204.4$ (4) Å^3, $Z = 4$, $D_m = 1.12$, $D_x = 1.19$ Mg m^{-3}, $\lambda(Mo\ K\alpha) = 0.71069$ Å, $\mu = 0.29$ mm^{-1}, $F(000) = 464$, $T = 293$ K, final $R = 0.062$ for 1261 unique observed reflections. There are two independent molecules in the asymmetric unit with identical geometries (within the limits of experimental error). The propoxy side chain is in a fully extended conformation (*i.e.* the arrangement of the ether O atom and the protonated amino group is *gauche*) and approximately perpendicular to the plane of the phenyl ring. The positive charge of the cations is compensated by three neighbouring chloride anions; two of the three $N^+ - H$ moieties donate their protons to different Cl^- anions, with $N^+ \cdots Cl^-$ distances ranging from 3.001 to 3.175 (7) Å, while the third is involved in bifurcated hydrogen bonding with the ether O atom (within the same molecule) and another Cl^- ion.

Introduction. The title compound (trivial name mexiletine) is an anti-arrhythmic agent belonging to the I*b* category, with considerable local anaesthetic activity (Remko & Mackov, 1990). The present structure determination is part of our programme to study structure–activity relationships in local anaesthetics.

Experimental. Single crystals from butanol, crystal used $0.4 \times 0.2 \times 0.1$ mm, D_m by flotation. Weissenberg photographs did not exhibit any symmetry. Lattice parameters refined on diffractometer from the positional angles of 16 reflections, $4 < 2\theta < 15°$. Intensity measurements on Syntex $P2_1$ diffractometer and graphite-monochromated Mo $K\alpha$ radiation. Correction for Lorentz and polarization factors using $XP2_1$ (Pavelčik, 1987), corrections for absorption and extinction neglected. Intensities of reflections in the range $0 < 2\theta \le 55°$ using θ–2θ scanning mode, each reflection scanned 1° (in 2θ) above and below $K\alpha$ doublet, background-to-scan-time ratio 1.0. Two standard reflections ($0\bar{1}\bar{1}$, $\bar{2}11$) every 98 reflections, 5354 unique reflections, $R_{int} = 0.027$, 1283 with $I \ge 1.96\sigma(I)$ considered observed and 1261 included in the refinement ($|\Delta F|/|F_o| < 0.53$). Index ranges h 0–11, k – 12–13, l – 17–18.

The structure was solved by the heavy-atom method in the space group $P\bar{1}$ using *SHELXS*86 (Sheldrick, 1986). Refinement on $|F_o|$ by a block-diagonal least-squares method, anisotropic thermal parameters for non-H atoms, only coordinates and thermal parameters of nine H atoms found in the difference Fourier map were refined; the remaining H atoms fixed at calculated positions, with the thermal parameters set to 0.5 higher than B_{eq} of the associated C or N atoms. Function minimized

Table 1. *Final atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal parameters,* B_{eq} (Å^2), *with e.s.d.'s in parentheses*

$$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Cl(1)	681 (3)	3309 (2)	1243 (2)	4·78 (10)
Cl(2)	2772 (3)	9517 (2)	9823 (2)	3·92 (9)
O(1)	−653 (6)	7737 (5)	2224 (4)	4·19 (22)
O(2)	4017 (6)	8362 (5)	2427 (4)	3·94 (21)
N(1)	411 (7)	7757 (6)	290 (4)	3·84 (29)
N(2)	3754 (7)	10847 (6)	1356 (4)	3·82 (26)
C(1)	−968 (10)	8153 (8)	3121 (5)	4·07 (36)
C(2)	−1307 (11)	7265 (9)	3886 (6)	5·69 (42)
C(3)	−1725 (11)	7716 (10)	4774 (6)	6·60 (50)
C(4)	−1756 (13)	8979 (11)	4865 (7)	8·06 (57)
C(5)	−1378 (11)	9838 (9)	4077 (7)	6·52 (43)
C(6)	−993 (10)	9434 (7)	3190 (6)	4·06 (35)
C(7)	−1325 (13)	5910 (9)	3829 (7)	7·19 (52)
C(8)	−581 (11)	10339 (8)	2310 (7)	5·36 (41)
C(9)	1033 (10)	7032 (8)	1949 (6)	4·44 (36)
C(10)	1152 (10)	6542 (8)	1021 (6)	4·23 (33)
C(11)	2856 (11)	5814 (8)	631 (7)	5·70 (38)
C(12)	4682 (10)	6968 (7)	2700 (5)	3·43 (32)
C(13)	5884 (9)	6198 (8)	2075 (6)	3·87 (35)
C(14)	6457 (10)	4806 (8)	2312 (6)	4·36 (37)
C(15)	5863 (10)	4205 (8)	3171 (6)	4·84 (36)
C(16)	4684 (10)	4975 (8)	3808 (6)	4·92 (39)
C(17)	4104 (10)	6392 (8)	3554 (5)	3·93 (33)
C(18)	6505 (11)	6843 (9)	1138 (6)	5·72 (44)
C(19)	2826 (11)	7250 (9)	4232 (6)	5·89 (41)
C(20)	4868 (10)	9141 (7)	2681 (6)	4·14 (37)
C(21)	3866 (10)	10586 (8)	2413 (5)	3·53 (35)
C(22)	4564 (11)	11582 (8)	2630 (6)	5·68 (45)

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

O(1)—C(1)	1·38 (1)	C(6)—C(8)	1·50 (1)
O(1)—C(9)	1·42 (1)	C(9)—C(10)	1·48 (1)
O(2)—C(12)	1·38 (1)	C(10)—C(11)	1·48 (1)
O(2)—C(20)	1·43 (1)	C(12)—C(13)	1·38 (1)
N(1)—C(10)	1·51 (1)	C(12)—C(17)	1·35 (1)
N(2)—C(21)	1·49 (1)	C(13)—C(14)	1·37 (1)
C(1)—C(2)	1·36 (1)	C(13)—C(18)	1·48 (1)
C(1)—C(6)	1·37 (1)	C(14)—C(15)	1·37 (1)
C(2)—C(3)	1·38 (1)	C(15)—C(16)	1·38 (1)
C(2)—C(7)	1·46 (1)	C(16)—C(17)	1·39 (1)
C(3)—C(4)	1·36 (1)	C(17)—C(19)	1·50 (1)
C(4)—C(5)	1·37 (1)	C(20)—C(21)	1·48 (1)
C(5)—C(6)	1·36 (1)	C(21)—C(22)	1·50 (1)

C(1)—O(1)—C(9)	113·9 (6)	C(5)—C(6)—C(8)	121·7 (8)
C(12)—O(2)—C(20)	114·7 (6)	O(1)—C(9)—C(10)	107·5 (7)
O(1)—C(1)—C(2)	116·6 (7)	N(1)—C(10)—C(9)	108·6 (7)
O(1)—C(1)—C(6)	119·3 (7)	N(1)—C(10)—C(11)	108·4 (7)
C(2)—C(1)—C(6)	123·9 (8)	C(9)—C(10)—C(11)	113·5 (7)
C(1)—C(2)—C(3)	116·7 (9)	O(2)—C(12)—C(13)	118·7 (7)
C(1)—C(2)—C(7)	125·0 (9)	O(2)—C(12)—C(17)	119·3 (7)
C(3)—C(2)—C(7)	118·3 (9)	C(13)—C(12)—C(17)	121·9 (8)
C(2)—C(3)—C(4)	120·7 (9)	C(12)—C(13)—C(14)	118·8 (8)
C(3)—C(4)—C(5)	121·0 (9)	C(12)—C(13)—C(18)	121·4 (7)
C(4)—C(5)—C(6)	119·8 (9)	C(14)—C(13)—C(18)	119·7 (8)
C(1)—C(6)—C(5)	117·9 (8)	C(13)—C(14)—C(15)	119·8 (8)
C(1)—C(6)—C(8)	120·4 (7)	C(14)—C(15)—C(16)	121·5 (8)
C(15)—C(16)—C(17)	117·9 (8)	O(2)—C(20)—C(21)	105·5 (6)
C(12)—C(17)—C(16)	119·9 (8)	N(2)—C(21)—C(20)	108·8 (6)
C(12)—C(17)—C(19)	121·1 (8)	N(2)—C(21)—C(22)	107·5 (7)
C(16)—C(17)—C(19)	119·0 (8)	C(20)—C(21)—C(22)	113·6 (7)

$\Sigma w(|F_o| - |F_c|)^2$ with $w^{-1} = \sigma^2(F_o) + (0·018|F_o|)^2$, where $\sigma(F_o)$ was derived from pulse statistics; final residual $R = 0·062$, $wR = 0·054$; in the last cycle
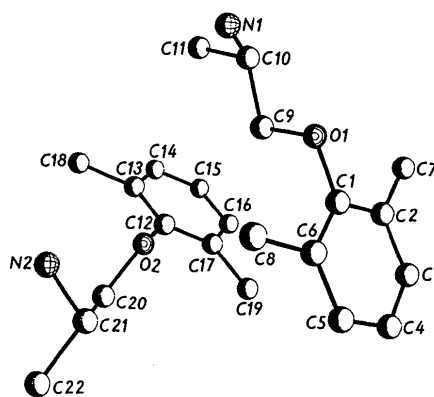

Fig. 1. A perspective view of the two symmetry-independent molecules of the title compound and numbering of the atoms.

$(\Delta/\sigma)_{max} = 0·048$, $(\Delta\rho)_{max} = 0·37$, $(\Delta\rho)_{min} = -0·28$ e Å^{-3}. All crystallographic calculations were carried out using the *XRC*83 (Pavelčík, Kettmann & Majer, 1985) program package.

Final crystallographic coordinates and equivalent B's of non-H atoms are listed in Table 1,* bond distances and angles in Table 2. A perspective view of two independent molecules is shown in Fig. 1 and gives the atom numbering.

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