C13—C14	1.398 (13)	1.384 (13)
C14—C15	1.391 (13)	1.393 (13)
C15—C16	1.408 (13)	1.404 (13)
C16—C17	1.362 (14)	1.372 (13)
	Molecule *C*	Molecule *D*
C1—C2	1.50 (2)	1.50(2)*/1.49(3)†
C2—C3	1.50 (2)	1.49(2)/1.47(4)
C2—O1	1.44 (1)	1.51(2)/1.38(4)

* Most occupied position. † Least occupied position.

Table 3. *Hydrogen-bonding geometry (Å, °)*

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O3*A*^{i}	0.91	2.11	2.89 (1)	143
N1*A*—H1*A*···O4*A*^{i}	0.91	2.30	3.14 (1)	152
N1*A*—H2*A*···O3*B*	0.91	1.86	2.77 (1)	175
N1*A*—H3*A*···O1*D*^{ii}	0.91	1.97	2.81 (1)	152
N2*A*—H6*A*···O2*B*^{iii}	0.88	2.09	2.95 (1)	165
N3*A*—H17*A*···O1*B*	0.88	2.12	2.97 (1)	163
N1*B*—H1*B*···O3*B*^{iv}	0.91	2.32	3.03 (1)	134
N1*B*—H1*B*···O4*B*^{iv}	0.91	1.91	2.74 (1)	151
N1*B*—H2*B*···O3*A*	0.91	2.11	2.80 (1)	132
N1*B*—H3*B*···O1*C*	0.91	2.05	2.80 (1)	140
N2*B*—H6*B*···O2*A*^{v}	0.88	2.00	2.84 (1)	159
N3*B*—H17*B*···O1*A*	0.88	2.18	3.05 (1)	172
O5*A*—H25*A*···O1*E*^{vi}	0.84	2.01	2.84 (1)	171
O5*B*—H25*B*···O1*G*	0.84	2.02	2.70 (1)	137
O1*C*—H8*C*···O1*H*	0.84	2.04	2.83 (1)	157
O1*E*—H1*E*···O1*F*	1.05	2.11 (12)	2.89 (1)	128 (9)
O1*G*—H1*G*···O2*A*	0.97	2.34 (17)	2.96 (1)	121 (13)

Symmetry codes: (i) $x, y, z-1$; (ii) $x-1, y, z-1$; (iii) $x-1, y, z$; (iv) $x, y, 1+z$; (v) $1+x, y, z$; (vi) $x, y-1, z$.

Table 4. *Molecular conformations (°) for Gly-L-Leu-L-Tyr in crystal structures*

Torsion angle	2-Propanol solvate*		DMSO solvate†		Cu complex‡	
	A	*B*	*A*	*B*	*A*	*B*
Backbones§						
ψ_1	156.6 (7)	169.5 (7)	154	170	−176	180
ω_1	177.7 (7)	178.5 (7)	−179	177	−177	−173
φ_2	−149.3 (7)	−123.5 (8)	−146	−132	−131	−130
ψ_2	132.7 (7)	143.6 (7)	135	148	142	139
ω_2	177.5 (7)	173.1 (7)	176	174	177	−177
φ_3	−129.7 (8)	−145.5 (7)	−140	−146	−142	−149
ψ_T	−13.4 (10)	−6.7 (11)	−10	−10	−23	−20
Side chains						
χ_2^1	−179.5 (7)	−55.0 (10)	−176	−60	176	−53
$\chi_2^{2,1}$	153.1 (9)	169.1 (8)	151	169	153	174
$\chi_2^{2,2}$	−83.8 (10)	−67.6 (10)	−86	−71	−92	−67
χ_3^1	65.0 (9)	65.2 (9)	59	66	58	54
$\chi_3^{2,1}$	86.2 (9)	−86.8 (9)	88	−88	84	−79
$\chi_3^{2,2}$	−94.8 (9)	98.0 (9)	−89	99	−86	90

* This work. † Subramanian & Parthasarathy (1987). ‡ Franks & van der Helm (1970). § ψ_1 = N1–C1–C2–N2, ω_1 = C3–N2–C2–C1, φ_2 = C2–N2–C3–C8, ψ_2 = N2–C3–C8–N3, ω_2 = C9–N3–C8–C3, φ_3 = C8–N3–C9–C10, ψ_T = N3–C9–C10–O3, χ_2^1 = N2–C3–C4–C5, $\chi_2^{2,1}$ = C3–C4–C5–C6, $\chi_2^{2,2}$ = C3–C4–C5–C7, χ_3^1 = N3–C9–C11–C12, $\chi_3^{2,1}$ = C9–C11–C12–C13, $\chi_3^{2,2}$ = C9–C11–C12–C17.

The structure was solved by direct methods using *SIR*92 (Altomare *et al.*, 1992) and refined with *SHELXL*93 (Sheldrick, 1993). All heavy atoms, except C and amide N backbone atoms and the disordered 2-propanol C atoms, were refined anisotropically. H atoms with known geometry were added in theoretical positions. The coordinates for the H atoms 'ride' on the coordinates of the corresponding heavy atom. Isotropic temperature factors for amino, hydroxyl and methyl H atoms were fixed to 1.5 times U_{eq} of the bonded heavy atom. Isotropic temperature factors for the remaining H atoms were fixed to 1.2 times U_{eq} of the attached heavy atom. The coordinates of the hydroxyl H atoms for the two Tyr residues and the two 2-propanol molecules were refined using a 'rotating group refinement' constraint with O—H = 0.84 Å. Three of the H atoms in the water molecules were located from the difference Fourier map, and their positions refined. Two alternative positions have been refined for the C atoms C1*D* and C2*D*, with occupancy factors 0.66 (3) for the pair C1*D*2 and C2*D*2, and 0.34 (3) for C1*D*1 and C2*D*1.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1338). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A. & Polidori, G. (1994). *J. Appl. Cryst.* **27**, 435.

Franks, W. A. & van der Helm, D. (1970). *Acta Cryst.* B**27**, 1299–1310.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Sheldrick, G. M. (1993). *SHELXL*93. *Program for Crystal Structure Refinement*. University of Göttingen, Germany.

Subramanian, E. & Parthasarathy, R. (1987). *Curr. Sci.* **56**, 1210–1213.

Wu, S., Tinant, B., Declercq, J.-P. & Van Meerssche, M. (1987). *Bull. Soc. Chim. Belg.* **96**, 275–280.

Acta Cryst. (1996). C**52**, 2090–2092

1-Phenyl-2-(propylamino)pentane, a Memory Enhancer

KÁLMÁN SIMON,[a] VERONIKA HARMAT,[b] ZOLTÁN TÖRÖK,[a] ZSOLT BÖCSKEI[a]* AND ISTVÁN HERMECZ[a]

[a]*Department of Chemical Research, Chinoin Pharmaceuticals, POB 110, 1325 Budapest, Hungary, and* [b]*Department of Theoretical Chemistry, Eötvös University, POB 32, 1518 Budapest, Hungary. E-mail: zsolt@para.chem.elte.hu*

(*Received 14 February 1996; accepted 19 April 1996*)

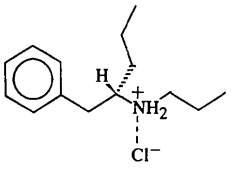
Abstract

The absolute configuration of [(*R*)-1-phenyl-2-pentyl]-propylammonium chloride, $C_{14}H_{24}N^+.Cl^-$, has been determined. The compound is a memory enhancer. Since the pharmacological effect of the related compound selegiline is highly dependent upon its configuration, the

title compound may be expected to behave in a similar manner.

Comment

Selegiline has been widely used in the treatment of Parkinson's disease. A number of similar compounds have been synthesized over the past few years. Of these we now describe the structure of [(*R*)-1-phenyl-2-pentyl]propylammonium chloride, (1), which is reported to facilitate learning and retention (Knoll, Knoll, Török, Timár & Yasar, 1992; Knoll & Miklya, 1994). Whereas amphetamines facilitate performance in a very narrow low dosage range which changes at a modest elevation of the dose into the opposite effect, compound (1) improves performance within a reasonably broad range. In the case of selegiline, the *R* enantiomer has much better pharmacological properties than its *S* counterpart (Robinson, 1985; Magyar, Vizi, Ecsery & Knoll, 1967). Therefore, we believe that an accurate characterization of these compounds is vitally important.



(1)

The crystal structure of (1) contains two crystallographically independent molecules in the asymmetric unit (Fig. 1). Both of these molecules are in the *R* configuration. The conformations of the two species are different, however, particularly with regard to the aliphatic side chains (Fig. 2). As far as the crystal packing is concerned, it is worth noting that parallel chains of hydrogen bonds formed by the chloride anions and the alkylammonium cations pack into hydrophilic layers in the *ab* plane (Fig. 3). This layer-like hydrogen-bond network is probably the most important contributor to intermolecular interactions. In between the hydrophilic layers there are hydrophobic layers packed with phenyl groups in the middle (Fig. 3).

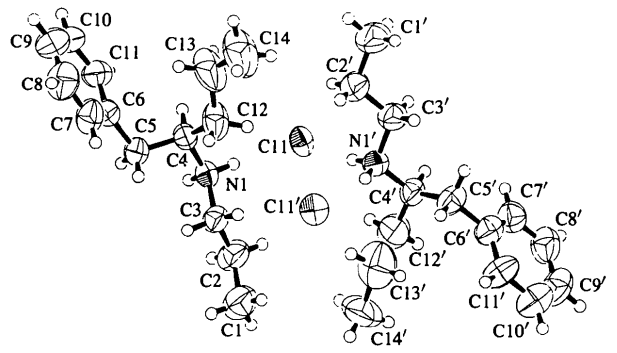


Fig. 1. The molecular structure and atomic numbering for (1). Displacement ellipsoids are plotted at the 50% probability level.

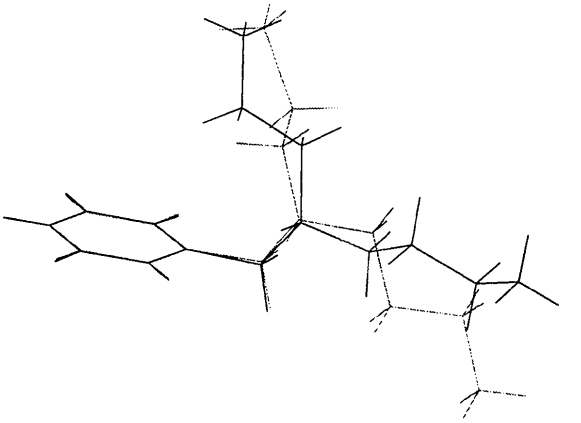


Fig. 2. Superposition of the two conformationally different molecules in the asymmetric unit.

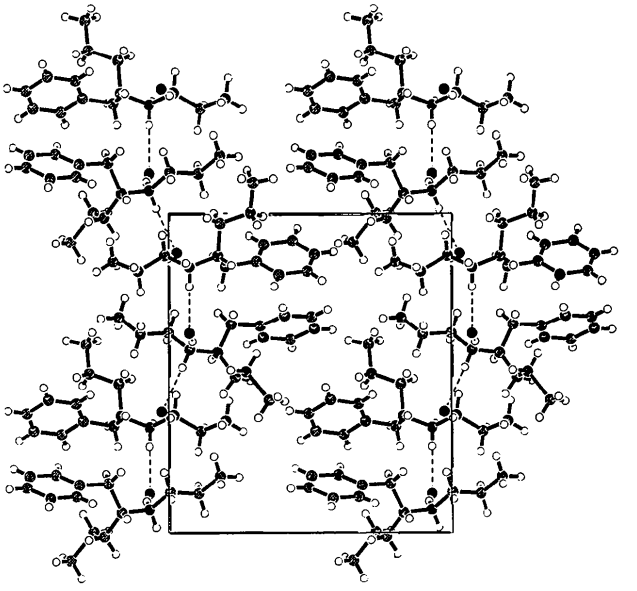


Fig. 3. A packing diagram for compound (1).

Experimental

The title compound was prepared according to Knoll, Knoll, Török, Timár & Yasar (1992) and Knoll *et al.* (1988, 1989).

Crystal data

$C_{14}H_{24}N^+.Cl^-$
M_r = 241.79
Monoclinic
$P2_1$
a = 7.665 (1) Å
b = 14.816 (1) Å
c = 13.237 (1) Å
β = 93.830 (1)°
V = 1500.0 (2) Å^3
Z = 4
D_x = 1.071 Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation
λ = 1.5418 Å
Cell parameters from 25 reflections
θ = 41.05–49.80°
μ = 2.050 mm^{-1}
T = 296 (2) K
Plate
0.25 × 0.20 × 0.11 mm
Transparent

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3222 measured reflections
3222 independent reflections
2186 observed reflections [$I > 2\sigma(I)$]
$\theta_{max} = 75.04°$
$h = 0 \rightarrow 9$
$k = -18 \rightarrow 0$
$l = -16 \rightarrow 16$
3 standard reflections monitored every 150 reflections
intensity decay: 1.2%

Refinement

Refinement on F^2
$R(F) = 0.0528$
$wR(F^2) = 0.1654$
$S = 1.024$
3219 reflections
295 parameters
Only H-atom U's refined
$w = 1/[\sigma^2(F_o^2) + (0.1161P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.013$
$\Delta\rho_{max} = 0.482$ e Å^{-3}
$\Delta\rho_{min} = -0.264$ e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.0029 (10)
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983) parameter = 0.00 (3)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
Cl1	−0.56763 (12)	1.12060 (7)	1.02645 (9)	0.0655 (3)
N1	−0.9531 (4)	1.1664 (3)	1.0732 (3)	0.0575 (8)
C1	−1.1422 (10)	1.1485 (6)	0.8000 (5)	0.106 (2)
C2	−1.0233 (8)	1.1790 (5)	0.8896 (4)	0.088 (2)
C3	−1.0657 (6)	1.1300 (4)	0.9856 (3)	0.0668 (11)
C4	−0.9866 (6)	1.1320 (3)	1.1754 (3)	0.0620 (11)
C5	−1.1690 (6)	1.1636 (4)	1.2017 (3)	0.0736 (13)
C6	−1.2084 (6)	1.1480 (3)	1.3109 (4)	0.0638 (11)
C7	−1.3463 (7)	1.0945 (4)	1.3353 (5)	0.082 (2)
C8	−1.3804 (10)	1.0821 (5)	1.4349 (6)	0.104 (2)
C9	−1.2815 (10)	1.1250 (7)	1.5107 (5)	0.102 (2)
C10	−1.1491 (9)	1.1785 (6)	1.4873 (4)	0.096 (2)
C11	−1.1100 (7)	1.1898 (5)	1.3882 (4)	0.0782 (14)
C12	−0.9539 (9)	1.0311 (4)	1.1845 (5)	0.094 (2)
C13	−0.8961 (15)	0.9990 (9)	1.2907 (8)	0.163 (5)
C14	−0.8464 (17)	0.9069 (8)	1.3015 (10)	0.175 (5)
Cl1′	−0.96329 (15)	0.87549 (8)	0.92696 (10)	0.0736 (3)
N1′	−0.5602 (5)	0.9271 (2)	0.9280 (3)	0.0580 (8)
C1′	−0.4018 (13)	0.8230 (6)	1.1814 (5)	0.117 (3)
C2′	−0.5212 (9)	0.8765 (6)	1.1046 (4)	0.093 (2)
C3′	−0.4514 (7)	0.8723 (4)	1.0033 (4)	0.0763 (13)
C4′	−0.4760 (7)	0.9362 (3)	0.8285 (4)	0.0638 (11)
C5′	−0.4508 (8)	0.8451 (4)	0.7806 (4)	0.0748 (13)
C6′	−0.3715 (7)	0.8500 (3)	0.6785 (4)	0.0719 (13)
C7′	−0.2116 (7)	0.8866 (4)	0.6684 (4)	0.0813 (14)
C8′	−0.1411 (9)	0.8926 (5)	0.5754 (5)	0.096 (2)
C9′	−0.2339 (12)	0.8588 (6)	0.4915 (6)	0.108 (2)
C10′	−0.3914 (12)	0.8215 (6)	0.5004 (5)	0.107 (2)
C11′	−0.4602 (10)	0.8179 (5)	0.5940 (4)	0.093 (2)
C12′	−0.5500 (13)	1.0115 (7)	0.7657 (6)	0.121 (3)
C13′	−0.7091 (12)	0.9961 (9)	0.7268 (9)	0.146 (4)
C14′	−0.7691 (12)	1.0853 (8)	0.6457 (7)	0.137 (3)

Table 2. *Selected geometric parameters (Å, °)*

N1—C4	1.484 (6)	N1′—C3′	1.496 (6)
N1—C3	1.499 (6)	N1′—C4′	1.511 (6)
C4—N1—C3	117.2 (4)	C3′—N1′—C4′	112.2 (4)
C1—C2—C3—N1	−176.5 (5)		
C4—N1—C3—C2	174.9 (4)		
C3—N1—C4—C5	−65.8 (5)		
C12—C4—C5—C6	64.0 (7)		
N1—C4—C5—C6	−169.6 (5)		
C5—C4—C12—C13	−84.4 (8)		
C4—C12—C13—C14	−173.7 (9)		
C1′—C2′—C3′—N1′	−177.5 (6)		
C4′—N1′—C3′—C2′	170.8 (5)		
C3′—N1′—C4′—C5′	60.7 (6)		
C12′—C4′—C5′—C6′	44.2 (9)		
N1′—C4′—C5′—C6′	178.3 (4)		
C5′—C4′—C12′—C13′	61.9 (10)		
C4′—C12′—C13′—C14′	−174.4 (6)		

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: *CAD*-4 *Software*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *TEXSAN* (Molecular Structure Corporation, 1985, 1992). Software used to prepare material for publication: *SHELXL*93.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, complete geometry and torsion angles have been deposited with the IUCr (Reference: KA1192). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Enraf–Nonius (1989). *CAD*-4 *Software*. Version 5. Enraf–Nonius, Delft, The Netherlands.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Knoll, J., Knoll, B., Török, Z., Timár, J. & Yasar, S. (1992). *Arch. Int. Pharmacodyn. Ther.* **316**, 5–29.

Knoll, J. & Miklya, I. (1994). *Arch. Int. Pharmacodyn. Ther.* **328**, 1–15.

Knoll, J., Simay, A., Szinnyei, É., Somfai, É., Török, Z., Mozsolits, K. & Bergmann, J. (1988). PCT Int. Appl. 88 02,254; *Chem. Abstr.* (1989). **110**, 128661.

Magyar, K., Vizi, E. Sz., Ecsery, Z. & Knoll, J. (1967). *Acta Physiol. Acad. Sci. Hung.* **32**, 377–387.

Molecular Structure Corporation (1985, 1992). *TEXSAN. TEXRAY Structure Analysis Package*. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

Robinson, B. J. (1985). *Biochem. Pharmacol.* **34**, 4105–4108.

Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.

Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.