Table 2. *Hydrogen bonding*

Superscripts refer to the following equivalent positions:

None	x,	y,	z	(iii)	$1 + x$, y, z
(i)	$-\frac{1}{2} + x$,	$1\frac{1}{2} - y$,	$\frac{1}{2} + z$	(iv)	$-1 + x$, y, z.
(ii)	$\frac{1}{2} + x$,	$1\frac{1}{2} - y$,	$-\frac{1}{2} + z$		

X–H$\cdots Y$	$X-Y$ (Å)	H$\cdots Y$ (Å)	$\angle X$–H$\cdots Y$ (°)
N(2)–H(2)$\cdots$N(8)	2·824 (4)	1·94 (3)	165 (3)
N(3)–H(3)$\cdots$N(4)	2·868 (4)	2·04 (3)	131 (2)
N(3)–H(4)$\cdots$O(2^{iii}) N(3^{iv})–H(4^{iv})$\cdots$O(2)	2·964 (3)	2·25 (3)	170 (4)
N(7)–H(12)$\cdots$N(1^{i}) N(7^{ii})–H(12^{ii})$\cdots$N(1)	2·813 (4)	1·88 (3)	177 (3)
N(9)–H(13)$\cdots$N(10)	2·908 (4)	2·29 (3)	132 (3)
N(9)–H(14)$\cdots$O(1^{iv}) N(9^{iii})–H(14^{iii})$\cdots$O(1)	2·960 (3)	2·08 (3)	166 (3)

Similar strong hydrogen bonds occur in imidazole (Craven *et al.*, 1977) where the N–H$\cdots$N distance is 2·86 Å compared with values of 2·83 and 2·81 Å in the present structure. Cross linking between the chains of DTIC molecules is provided by pairs of hydrogen bonds between amide groups [N(3)–H$\cdots$O(2) and N(9)–H$\cdots$O(1)]. In the directions normal to the planes of the imidazole rings there are no contacts shorter than 3·5 Å with neighboring molecules.

Results of the present work which may be relevant to the biological effects of DTIC are that (i) the side-chain configurations are not affected by changes in pH (since the same configurations are observed in crystals of DTIC and HDTIC$^+$ grown under quite different conditions and having different intermolecular interactions), and (ii) the shape of the imidazole ring undergoes subtle changes depending on whether one N(imidazole) atom or the other or both are protonated.

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The Crystal Structure of Phenylpropanolamine Hydrochloride (2-Amino-1-phenyl-1-propanol Hydrochloride)

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Abstract

(±)-Phenylpropanolamine or norephedrine hydrochloride, $C_9H_{14}NO^+.Cl^-$, crystallizes in the non-centrosymmetric space group $P2_1$. The unit-cell dimensions are $a = 14·519$ (10), $b = 9·456$ (3), $c = 7·433$ (9) Å, $\beta = 103·50$ (2)°. The structure was determined by the Patterson method and refined by a full-matrix least-squares procedure to an R value of 0·032 for 1756 statistically significant observed reflexions collected by diffractometry. The two optical isomers of the phenylpropanolamine molecule have different conformations in the crystal; one has an extended *trans* conformation while the other is folded into a *gauche* form. The hydrogen-bonded interactions, holding the structure together in the b and c directions, may have an important influence on the molecular conformations.

Introduction

Phenylpropanolamine is an adrenergic drug, widely used as an orally active nasal decongestant. Its vasoconstrictor potency is comparable to that of ephedrine.

However, ephedrine is more active than phenyl-propanolamine with respect to stimulation of the central nervous system (Goth, 1972). A recent investigation (Wikberg, 1978) shows that phenylpropanolamine has a pronounced selective effect on the postjunctional α receptor.

Experimental

The racemic mixture of the title compound was obtained from the pharmaceutical company AB Leo. The sample was recrystallized by evaporation of an aqueous solution. One optically perfect crystal was reshaped by partial dissolution to measure $0.4 \times 0.3 \times 0.2$ mm. Preliminary unit-cell dimensions and systematic absences were determined from Weissenberg photographs while accurate cell parameters were obtained from diffractometer data. The density was measured by flotation in a xylene–chloroform mixture.

Crystal data

Phenylpropanolamine (norephedrine or 2-amino-1-phenyl-1-propanol) hydrochloride, $C_9H_{14}NO^+.Cl^-$, $M_r = 187.67$, $a = 14.519$ (10), $b = 9.456$ (3), $c = 7.433$ (9) Å, $\beta = 103.50$ (2)°, $V = 992.29$ Å³, $D_m = 1.252$ (5), $D_x(Z = 4) = 1.256$ Mg m⁻³, $\mu(Mo\ K\alpha) = 0.337$ mm⁻¹.

Systematic absences: $0k0$ when k is odd, which gives two possible space groups, $P2_1$ and $P2_1/m$. The existence of a mirror plane perpendicular to the b axis was tested (Woolfson, 1970) by comparing $|F_{h0l}|^2$ and $|F_{hkl}|^2$ within $16.0° \le \theta \le 18.0°$. This test showed that the presence of a mirror plane in the structure was unlikely. Further support for the non-centrosymmetric space group $P2_1$ was obtained from E-value statistics. The choice of $P2_1$, with two isomers in the asymmetric unit, was fully confirmed by the structure determination.

The crystal was mounted about its b axis in an automatic linear diffractometer (Pailred). Integrated intensities for 2464 unique reflexions within $\sin \theta/\lambda \le 0.65$ Å⁻¹ ($hk0$ through $hk12$) were measured using graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0.7107$ Å). The fainter reflexions were scanned twice and the background was measured for 40 s at each end of the scan. Reference reflexions recorded at regular intervals during the data collection showed no significant changes. The measured intensities were corrected for Lorentz and polarization factors, but not for absorption because of the low μ value. At this stage 708 reflexions with intensities $I < 3.3\sigma(I)$ were excluded from further calculations. The remaining 1756 net amplitudes were placed on an approximately absolute scale by Wilson statistics.

Structure determination and refinement

In a three-dimensional Patterson map the peaks corresponding to the Cl atoms could be located. Five partially phased Fourier syntheses revealed the non-hydrogen atoms of the two phenylpropanolamine molecules. The refinement was carried out by a full-matrix least-squares procedure. Difference syntheses calculated during the refinement located all the H atoms and their positional parameters were introduced in the refinement. All H atoms were allotted an overall isotropic temperature factor $U = 0.05$ Å². The weighting scheme employed was $w = 1/[\sigma^2(F) + 0.001F^2]$, where $\sigma(F)$ is the standard deviation in the observed amplitudes based on counting statistics. The average positional-parameter shifts of the last cycle expressed as fractions of the e.s.d.'s were 0.077. The final R value ($R = \sum ||F_o| - |F_c||/\sum |F_o|$) was 0.032 for the 1756 statistically significant observed amplitudes. The atomic fractional coordinates are given in Tables 1 and 2. The atomic scattering factors were those of the SHELX system, also given in International Tables for X-ray Crystallography (1974). The computations were performed on an IBM 370/165 using the SHELX program system (Sheldrick, 1975) except for the initial data reduction and the Lorentz and polarization corrections which were carried out by our program system (Bergin, 1971a) and the stereo-

Table 1. *Final fractional coordinates* $(\times 10^4)$ *for non-hydrogen atoms*

E.s.d.'s are in parentheses in units of the last digit.

	x	y	z
Cl(1)	1487 (1)	2500 (0)	889 (1)
Cl(2)	58 (1)	331 (1)	5318 (1)
OA	9242 (2)	1660 (3)	1360 (4)
NA	9656 (2)	4484 (3)	426 (4)
C(1)A	6770 (3)	2906 (4)	725 (5)
C(2)A	5863 (3)	2379 (5)	110 (6)
C(3)A	5718 (3)	1083 (5)	9269 (7)
C(4)A	6478 (3)	301 (5)	9012 (5)
C(5)A	7388 (3)	832 (4)	9599 (5)
C(6)A	7544 (2)	2133 (3)	471 (4)
C(7)A	8531 (2)	2735 (3)	1100 (5)
C(8)A	8734 (3)	3771 (3)	9662 (5)
C(9)A	8771 (3)	3100 (4)	7819 (5)
OB	2609 (2)	1353 (3)	8084 (4)
NB	1462 (2)	2882 (3)	5127 (4)
C(1)B	3179 (3)	555 (4)	4963 (5)
C(2)B	3588 (3)	27 (4)	3610 (6)
C(3)B	4321 (4)	763 (6)	3123 (7)
C(4)B	4629 (3)	1993 (6)	3993 (7)
C(5)B	4218 (3)	2536 (5)	5334 (6)
C(6)B	3473 (2)	1834 (4)	5816 (5)
C(7)B	3012 (3)	2467 (4)	7257 (4)
C(8)B	2255 (3)	3578 (3)	6487 (5)
C(9)B	2598 (3)	4863 (4)	5597 (6)

views which were produced by the plotting program *ORTEP* (Johnson, 1965).*

Description of the structure

The geometry of the molecules

The numbering of the atoms in the two molecules in the asymmetric unit is shown in Fig. 1 and intra-molecular bond lengths and angles, uncorrected for thermal motion, are given in Table 3. Corresponding interatomic distances and angles between non-hydrogen atoms are very similar in both molecules and show no significant deviations from standard values except for the slightly distorted tetrahedral arrangement around the α C(8) atom. Thus the angle C(7)–C(8)–C(9) is greater than the expected tetrahedral value in both molecules. This is probably due to interaction with the neighbouring OH group. Similar

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34328 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Final fractional coordinates* (×10³) *for hydrogen atoms having a temperature factor U of* 0·05 Å²

E.s.d.'s are in parentheses in units of the last digit.

	x	y	z
H(1)A	688 (3)	369 (5)	133 (6)
H(2)A	534 (3)	298 (5)	46 (5)
H(3)A	504 (3)	73 (4)	−117 (5)
H(4)A	638 (3)	−59 (5)	−154 (5)
H(5)A	791 (3)	39 (5)	−56 (5)
H(7)A	859 (3)	321 (5)	227 (5)
H(O)A	930 (3)	137 (5)	243 (6)
H(8)A	826 (3)	442 (5)	−63 (5)
H(9A)A	939 (3)	251 (5)	−207 (5)
H(9B)A	815 (2)	268 (5)	−280 (5)
H(9C)A	880 (3)	380 (5)	−299 (6)
H(NA)A	11 (3)	386 (5)	44 (6)
H(NB)A	968 (3)	516 (4)	−16 (6)
H(NC)A	962 (3)	473 (5)	154 (6)
H(1)B	736 (3)	515 (5)	470 (6)
H(2)B	666 (3)	408 (5)	701 (6)
H(3)B	531 (3)	533 (5)	790 (5)
H(4)B	489 (3)	734 (5)	638 (6)
H(5)B	561 (3)	845 (4)	404 (6)
H(7)B	643 (3)	799 (4)	184 (6)
H(O)B	239 (3)	153 (5)	882 (6)
H(8)B	804 (3)	893 (5)	258 (5)
H(9A)B	794 (3)	47 (5)	−523 (5)
H(9B)B	717 (3)	−44 (5)	−460 (5)
H(9C)B	688 (3)	24 (5)	−644 (5)
H(NA)B	100 (3)	350 (5)	484 (6)
H(NB)B	166 (3)	262 (5)	395 (5)
H(NC)B	873 (3)	700 (5)	429 (5)

distortions are also found in structures of ephedrine compounds, ephedrine hydrochloride (Bergin, 1971*b*), ephedrine monohydrogen phosphate monohydrate (Hearn, Freeman & Bugg, 1973) and ephedrine dihydrogen phosphate (Hearn & Bugg, 1972) but not in pseudoephedrine and pseudoephedrine hydrochloride (Mathew & Palenik, 1977), where the *threo* configuration gives a larger C(9)···O distance.

The bonds involving H atoms are all quite normal and corresponding bond angles have a maximal deviation of about 10° from expected values.

Table 3. *Intermolecular bond distances* (Å) *and angles* (°) *with estimated standard deviations in parentheses*

C(1)A–C(2)A	1·383 (6)	C(1)B–C(2)B	1·375 (6)
C(2)A–C(3)A	1·370 (7)	C(2)B–C(3)B	1·389 (7)
C(3)A–C(4)A	1·378 (7)	C(3)B–C(4)B	1·355 (8)
C(4)A–C(5)A	1·385 (5)	C(4)B–C(5)B	1·375 (6)
C(5)A–C(6)A	1·384 (4)	C(5)B –C(6)B	1·386 (5)
C(6)A–C(1)A	1·390 (5)	C(6)B–C(1)B	1·386 (5)
C(6)A–C(7)A	1·511 (5)	C(6)B–C(7)B	1·513 (5)
C(7)A–OA	1·429 (4)	C(7)B–OB	1·413 (4)
C(7)A–C(8)A	1·528 (4)	C(7)B–C(8)B	1·531 (5)
C(8)A–C(9)A	1·522 (5)	C(8)B–C(9)B	1·522 (5)
C(8)A–NA	1·489 (4)	C(8)B–NB	1·496 (5)

|			
C(6)A–C(1)A–C(2)A	120·3 (3)	C(6)B–C(1)B–C(2)B	120·8 (4)
C(1)A–C(2)A–C(3)A	120·4 (4)	C(1)B–C(2)B–C(3)B	119·8 (4)
C(2)A–C(3)A–C(4)A	120·0 (4)	C(2)B–C(3)B–C(4)B	119·6 (4)
C(3)A–C(4)A–C(5)A	119·9 (4)	C(3)B–C(4)B–C(5)B	121·0 (4)
C(4)A–C(5)A–C(6)A	120·6 (4)	C(4)B–C(5)B–C(6)B	120·4 (4)
C(5)A–C(6)A–C(1)A	118·8 (3)	C(5)B–C(6)B–C(1)B	118·4 (4)
C(5)A–C(6)A–C(7)A	121·3 (3)	C(5)B–C(6)B–C(7)B	119·6 (3)
C(1)A–C(6)A–C(7)A	119·9 (3)	C(1)B–C(6)B–C(7)B	122·0 (3)
C(6)A–C(7)A–OA	112·1 (3)	C(6)B–C(7)B–OB	108·0 (3)
C(6)A–C(7)A–C(8)A	110·4 (3)	C(6)B–C(7)B–C(8)B	113·8 (3)
OA–C(7)A–C(8)A	107·4 (3)	OB–C(7)B–C(8)B	109·9 (3)
C(7)A–C(8)A–C(9)A	114·5 (3)	C(7)B–C(8)B–C(9)B	115·6 (3)
C(7)A–C(8)A–NA	109·1 (3)	C(7)B–C(8)B–NB	108·9 (3)
C(9)A–C(8)A–NA	108·3 (3)	C(9)B–C(8)B–NB	109·6 (3)
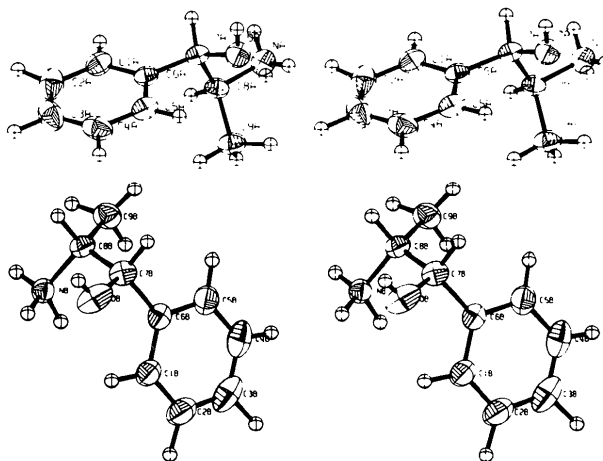
Fig. 1. Stereoscopic drawings of the phenylpropanolamine molecules as seen along *b*. Heavy atoms are represented by thermal ellipsoids of 50% probability. Hydrogen atoms are depicted as small spheres.

As can be seen from the stereoscopic pairs in Fig. 1 the two isomers of phenylpropanolamine have different conformations in the crystal. The A molecule has a maximally extended *trans* conformation with an anti-periplanar torsion angle τ_2, C(6)—C(7)—C(8)—N, of 172·7 (4)°, whereas the B molecule is folded into a *gauche* conformation resulting in a τ_2 angle of 63·6 (4)°. These conformations correspond to those found in a quantum-mechanical study of phenylpropanolamine (Pullman, Coubeils, Courrière & Gervois, 1972). In these calculations, carried out utilizing the PCILO method, two regions of stability were found: a global minimum corresponding to an extended conformation and a local minimum, about 4 kJ mol^{-1} above the global one, corresponding to a folded form. As the energy barrier separating these conformations is so low it may be expected that external conditions like crystal packing forces will have an important influence on the molecular conformation. However, quantum-mechanical calculations (Kier, 1968, 1969, 1971; Pullman, Coubeils, Courrière & Gervois, 1972), NMR

studies (Portoghese, 1967; Bustard & Egan, 1971; Neville, Deslauriers, Blackburn & Smith, 1971) and crystal structure determinations (Bergin, 1971c; Hearn, Freeman & Bugg, 1973; Carlström, Bergin & Falkenberg, 1973) of a large number of phenethylamine derivatives show a pronounced preference for the *trans* conformation.

The torsion angles τ_1, C(5)A—C(6)A—C(7)A—C(8)A in molecule A and C(1)B—C(6)B—C(7)B—C(8)B in molecule B, are 97·0 (4) and −97·1 (4)° respectively. Least-squares planes were calculated for the benzene rings of both molecules and the ethylamine side chain of molecule A. As can be seen in Table 4 the maximum deviation of an individual atom in the phenyl rings is 0·015 Å and of an atom in the side chain 0·046 Å.

Hydrogen bonds and molecular packing

All protons of the N and the hydroxyl group of both molecules participate in the hydrogen-bonding system where each Cl ion acts as acceptor for four hydrogen bonds. Two types of hydrogen bonds (Table 5), N—H···Cl and O—H···Cl, form continuous layers parallel to (100) with the phenylpropanolamine cations extending perpendicularly along the a axis. Apart from this hydrogen-bonding system the structure is held together by van der Waals forces between the hydrophobic parts of the molecules. A stereoview of the molecular packing is shown in Fig. 2.

In molecule A the distance between the charged NA atom and the OA atom is 2·859 Å. However, no H atom is available for the formation of a hydrogen bond between these two atoms.

Table 4. *Least-squares planes and deviations (Å) of individual atoms*

The equations of the planes are in the form $AX + BY + CZ = D$, where X, Y and Z are coordinates in orthogonal Ångström space along a, b and c respectively. E.s.d.'s are in parentheses in units of the last digit.

Plane of benzene ring (A)
$$-0.1369X - 0.4395Y + 0.8878Z = -2.0745$$

C(1)A	0·004 (4)	C(4)A	0·005 (4)
C(2)A	−0·006 (5)	C(5)A	−0·007 (4)
C(3)A	0·002 (5)	C(6)A	0·002 (3)

Plane of side chain (A)
$$0.5297X - 0.7389Y - 0.4169Z = 4.1722$$

C(6)A	−0·045 (3)	C(8)A	0·044 (4)
C(7)A	0·046 (3)	NA	−0·045 (3)

Plane of benzene ring (B)
$$0.5106X - 0.4977Y + 0.7011Z = 4.1581$$

C(1)B	0·013 (4)	C(4)B	0·006 (5)
C(2)B	−0·001 (4)	C(5)B	0·006 (6)
C(3)B	−0·008 (6)	C(6)B	−0·015 (4)

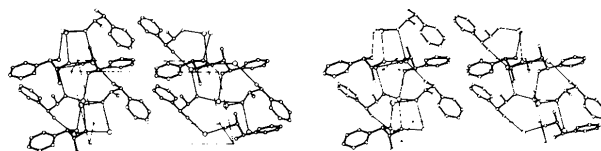Fig. 2. Stereoscopic drawing of the molecular packing as seen along b. Thin lines represent hydrogen bonds.

Table 5. *Hydrogen-bonded interactions*

The columns labelled x',y',z' give the symmetry of the acceptor atom Y'. The reference molecule is in x,y,z. E.s.d.'s are in parentheses in units of the last digit.

X	H	Y'	x'	y'	z'	$X \cdots Y'$	$H \cdots Y'$	$X-H \cdots Y'$
NA	H(NA)A	Cl(1)	$1 + x$	y	z	3·205 (3) Å	2·33 (5) Å	169 (1)°
NA	H(NB)A	Cl(1)	$1 - x$	$y + \frac{1}{2}$	$-z$	3·328 (3)	2·76 (4)	131 (1)
NA	H(NC)A	Cl(2)	$1 - x$	$y + \frac{1}{2}$	$1 - z$	3·195 (3)	2·35 (5)	165 (1)
OA	H(O)A	Cl(2)	$1 + x$	y	z	3·164 (3)	2·38 (5)	158 (1)
NB	H(NA)B	Cl(2)	$-x$	$y + \frac{1}{2}$	$1 - z$	3·161 (3)	2·30 (5)	168 (1)
NB	H(NB)B	Cl(1)	x	y	z	3·178 (3)	2·23 (4)	155 (1)
NB	H(NC)B	Cl(2)	x	y	z	3·183 (3)	2·33 (4)	141 (1)
OB	H(O)B	Cl(1)	x	y	$1 + z$	3·124 (3)	2·43 (5)	168 (1)

The hydrogen-bonding system and the packing arrangement may well explain the two different conformations of the phenylpropanolamine molecules of the structure.

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Syncrystallization of Enantiomers or Diastereoisomers.
I. Structure of (+)-(2R,αS)-2-Isopropyl-α-methyl-5-indanacetic Acid (C₁₅H₂₀O₂)

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Abstract

The structure of one optically active diastereoisomer of the anti-inflammant 2-isopropyl-α-methyl-5-indanacetic acid has been determined. With the aid of circular dichroism its relative and absolute configurations have been found. It crystallizes in space group $P2_12_12_1$ with $Z = 8$ (2 independent molecules), $a = 26.207$ (52), $b = 11.802$ (23), $c = 8.755$ (17) Å. $R = 5.8\%$ for 1549 structure factors $[I \geq 3\sigma(I)]$.

Introduction

2-Isopropyl-α-methyl-5-indanacetic acid, prepared as an inseparable mixture of the two racemic diastereo-
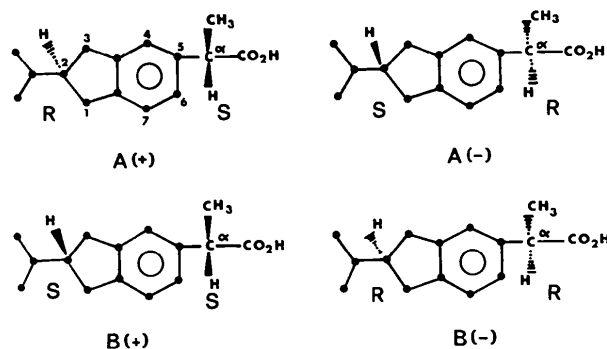
Fig. 1. Representation of the four isomers (two diastereoisomers) A (RS and SR) and B (SS and RR).