Table 5. *Details of the hydrogen bonds*

Donor *D*	Acceptor *A*	*D*···*A*	∠*D*–H···*A*	∠H–*D*···*A*
N(3)	O(2)*	2·904 (7) Å	156·9 (25)°	16·5 (20)°
N(1)	O(3)^{i}	2·997 (7)	144·5 (24)	27·2 (21)
N(2)	O(4)^{ii}	3·147 (8)	138·7 (24)	32·9 (22)

Symmetry code: superscript: (i) $1-x$, $1-(y+\frac{1}{2})$, $1-z$; (ii) $-x$, $1-(y+\frac{1}{2})$, $1-z$.

* Intramolecular hydrogen bond.

induces β-bend formation and the consequent generation of a 3_{10}-helical segment.

The crystal structure viewed along **b** is shown in Fig. 2. In addition to the good intramolecular NH···O hydrogen bond between the CO of the urethan moiety and NH of the alanyl residue, the other peptide NH and CO groups are involved in intermolecular hydrogen bonds. The details of the inter- and intramolecular hydrogen bonds are given in Table 5.

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The Crystal Structure of (+)-2-Dipropylamino-5-hydroxytetralin Hydrochloride

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Abstract

The title compound, $C_{16}H_{26}NO^+.Cl^-$, which is a potent dopaminergic drug, is monoclinic with $a = 7{\cdot}601$ (1), $b = 18{\cdot}508$ (3), $c = 11{\cdot}408$ (2) Å, $\beta = 94{\cdot}28$ (1)°, space group $P2_1$ and $Z = 4$. The structure was solved by direct methods and refined to $R = 0{\cdot}052$ for 2081 counter-measured observed reflections. The structure consists of infinite chains along the *b* axis, the molecules being connected by hydrogen-bonded chloride ions. Adjacent chains are held together by van de Waals forces only. The non-aromatic ring assumes a

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half-chair conformation with the N atom attached equatorially. The molecules of the title compound thus resemble the *trans* form of dopamine.

Introduction

In the study of the structure of biologically active amines, interest has for some years focused on so-called rigid analogues, *i.e.* substances where the originally flexible side chain is fixed by the introduction of new atoms into the molecule. Two good examples of such model substances are LSD and apomorphine. It is hoped that by examining a series of compounds where the chain is fixed in different conformations one may find the optimal structure for biological effect.

The best known rigid analogue of dopamine is apomorphine, whose structure was solved at this department (Giesecke, 1973, 1977). Another interesting group of dopamine analogues is the 2-aminotetralins (Fig. 1). Their pharmacological properties have been studied by a number of researchers, *e.g.* Cannon, Kim & Aleem (1972) and McDermed, McKenzie & Phillips (1975).

The non-aromatic ring of the aminotetralins is really only semi-rigid, and the main aim of this study was to find out if the N atom is attached equatorially, which would correspond to the *trans* form of dopamine shown by X-ray diffraction (Bergin & Carlström, 1968), or axially, resembling the *gauche* form of dopamine proposed by Kier & Truitt (1970) from EHT calculations. Furthermore, McDermed, McKenzie & Freeman (1976) found that only the (−) isomer of 2-amino-5-hydroxytetralin possesses any dopaminergic activity, and since Saari, King & Lotti (1973) have shown that only the (6a*R*)-(−) isomer of apomorphine is active, a comparison of these two substances seemed interesting.

An alternative name for a 2-aminotetralin is 2-amino-1,2,3,4-tetrahydronaphthalene, but since most pharmacologists seem to prefer the former denomination it will be used below (also abbreviated 2-AT).

Experimental

A sample of 2-dipropylamino-5-hydroxytetralin was kindly supplied by Dr McDermed, Wellcome Research Laboratories. As his stock of both enantiomers was very limited, only 5 mg of the inactive (+) form could be spared for a diffraction study. Luckily, a few crystals were immediately obtained from an aqueous solution left to evaporate at room temperature. The crystal chosen for study was a triangular prism with the edges of the pinacoids measuring 200, 300, and 300 μm respectively. The length of the prism was 500 μm.

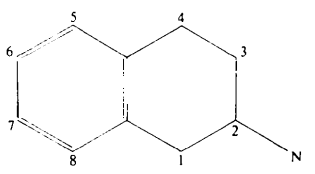

Fig. 1. The 2-aminotetralin skeleton with the chemical numbering scheme.

Crystal data

(+)-2-Dipropylamino-5-hydroxy-1,2,3,4-tetrahydronaphthalene hydrochloride, $C_{16}H_{26}NO^+.Cl^-$, monoclinic, $a = 7{\cdot}601\ (1)$, $b = 18{\cdot}508\ (3)$, $c = 11{\cdot}408\ (2)$ Å, $\beta = 94{\cdot}28\ (1)°$, $M_r = 283{\cdot}84$, $V = 1600{\cdot}4$ Å^3, $D_m = 1{\cdot}172\ (5)$, $D_x(Z = 4) = 1{\cdot}178$ Mg m^{-3}, $F(000) = 1004$, μ(Mo $K\alpha$) $= 0{\cdot}269$ mm^{-1}.

Systematic absences and the asymmetry of the 2-AT molecule singled out $P2_1$ as the only possible space group, the asymmetric unit containing two molecules.

The crystal was mounted around **b**, orthogonally to the smallest prism face. The integrated intensities were measured on a Pailred diffractometer, with graphite-monochromated Mo $K\alpha$ radiation ($\lambda = 0{\cdot}7107$ Å). Faint reflexions were scanned twice, and the background was measured for 20 s on each side. In this way the layers *h*0*l* through *h*24*l* were recorded, corresponding to $\sin\theta/\lambda < 0{\cdot}65$ Å^{-1}. Standard reflexions measured at regular intervals showed no significant change in intensity. Of the 4125 unique reflexions, 2044 had intensities not statistically different from the background level, and were thus excluded from further computations. The net intensities were corrected for Lorentz and polarization factors, but not for absorption owing to the low μ value. The corrected structure factor amplitudes were placed on an approximately absolute scale by Wilson statistics.

Structure determination and refinement

A three-dimensional Patterson map immediately indicated that the two independent Cl atoms occupied rather special positions in the cell, namely approximately (+0·25, *y*, 0·5) and (−0·25, *y* + 0·07, 0·0). This meant that the two sets of vectors between screw-related atoms very nearly coincided, and their exact *x* and *z* components could not be resolved properly. A Fourier synthesis based on the coarse coordinates above thus failed to show any new atoms unequivocally. 180 *E* values, including all *E*'s > 1·5, were therefore fed into the program *MULTAN* (Germain, Main & Woolfson, 1971). An *E* map from the best *MULTAN* set resolved the ambiguity of the Cl positions, and showed another nine peaks that could be fitted into a model of the 2-AT molecule. By two three-dimensional electron density calculations all 38 non-

Table 1. *Final fractional coordinates for all non-hydrogen atoms*

E.s.d.'s in parentheses are in units of the last digit. Rough B values in (Å^2) are calculated from the last refinement.

	x	y	z	B		x	y	z	B
Cl*A*	0·7600 (3)	0·7109	0·0118 (2)	3·7	Cl*B*	0·2687 (2)	0·7776 (1)	0·4970 (2)	6·0
N(1)*A*	0·3491 (8)	0·7023 (3)	−0·0285 (5)	3·7	N(1)*B*	0·8730 (6)	0·7730 (3)	0·4137 (5)	3·0
C(1)*A*	0·3503 (10)	0·9202 (4)	0·2294 (6)	3·9	C(1)*B*	0·4451 (9)	0·5745 (4)	0·4453 (7)	3·9
C(2)*A*	0·3279 (11)	0·9922 (4)	0·2471 (7)	4·6	C(2)*B*	0·4111 (9)	0·5023 (4)	0·4630 (6)	4·1
C(3)*A*	0·2746 (10)	1·0380 (4)	0·1518 (7)	3·9	C(3)*B*	0·5426 (10)	0·4526 (4)	0·4507 (6)	3·6
C(4)*A*	0·2401 (9)	1·0069 (4)	0·0429 (6)	3·6	C(4)*B*	0·7043 (9)	0·4746 (4)	0·4185 (6)	2·8
C(5)*A*	0·2649 (10)	0·9333 (4)	0·0236 (7)	3·4	C(5)*B*	0·7398 (9)	0·5474 (4)	0·3970 (6)	2·8
C(6)*A*	0·3199 (9)	0·8884 (4)	0·1189 (6)	3·3	C(6)*B*	0·6079 (9)	0·5977 (4)	0·4099 (6)	3·1
C(7)*A*	0·3470 (10)	0·8086 (4)	0·1046 (6)	4·0	C(7)*B*	0·6383 (10)	0·6768 (4)	0·3911 (7)	4·2
C(8)*A*	0·2717 (9)	0·7777 (4)	−0·0149 (6)	3·7	C(8)*B*	0·8329 (8)	0·6928 (4)	0·4166 (6)	2·6
C(9)*A*	0·3176 (11)	0·8281 (4)	−0·1123 (6)	4·1	C(9)*B*	0·9392 (9)	0·6492 (4)	0·3331 (6)	3·4
C(10)*A*	0·2270 (11)	0·9014 (4)	−0·0976 (7)	4·5	C(10)*B*	0·9218 (9)	0·5690 (4)	0·3647 (6)	3·5
C(11)*A*	0·2860 (10)	0·6504 (4)	0·0624 (7)	3·8	C(11)*B*	0·8228 (10)	0·8075 (4)	0·2971 (6)	3·8
C(12)*A*	0·3641 (12)	0·5750 (5)	0·0576 (8)	6·2	C(12)*B*	0·8979 (13)	0·8811 (5)	0·2806 (8)	5·5
C(13)*A*	0·2899 (15)	0·5239 (5)	0·1438 (8)	6·4	C(13)*B*	0·8451 (12)	0·9100 (5)	0·1600 (8)	5·6
C(14)*A*	0·3272 (11)	0·6713 (4)	−0·1511 (7)	4·3	C(14)*B*	0·7930 (9)	0·8140 (4)	0·5116 (6)	3·4
C(15)*A*	0·1380 (11)	0·6502 (4)	−0·1880 (7)	4·8	C(15)*B*	0·8358 (10)	0·7832 (4)	0·6352 (6)	4·5
C(16)*A*	0·1336 (13)	0·6115 (4)	−0·3060 (7)	5·9	C(16)*B*	0·7824 (13)	0·8345 (5)	0·7291 (8)	6·2
O(1)*A*	0·1794 (8)	1·0477 (3)	−0·0534 (5)	4·9	O(1)*B*	0·8406 (6)	0·4268 (3)	0·4190 (5)	4·4

Table 2. *Final fractional coordinates for all hydrogen atoms*

E.s.d.'s are in units of the last digit. $B = 4·0$ Å^2.

	x	y	z		x	y	z
H(1)*A*	0·376 (9)	0·889 (4)	0·300 (6)	H(1)*B*	0·356 (9)	0·612 (4)	0·449 (6)
H(2)*A*	0·346 (9)	1·012 (4)	0·329 (6)	H(2)*B*	0·291 (9)	0·479 (4)	0·483 (6)
H(3)*A*	0·261 (9)	1·090 (4)	0·160 (6)	H(3)*B*	0·522 (9)	0·406 (4)	0·474 (6)
H(7*A*)*A*	0·266 (9)	0·794 (4)	0·159 (6)	H(7*A*)*B*	0·569 (9)	0·714 (4)	0·429 (5)
H(7*B*)*A*	0·484 (9)	0·796 (4)	0·101 (6)	H(7*B*)*B*	0·604 (9)	0·696 (4)	0·312 (6)
H(8)*A*	0·157 (9)	0·781 (4)	−0·008 (6)	H(8)*B*	0·874 (9)	0·678 (4)	0·500 (6)
H(9*A*)*A*	0·299 (9)	0·802 (4)	−0·201 (6)	H(9*A*)*B*	1·045 (9)	0·668 (4)	0·342 (6)
H(9*B*)*A*	0·452 (9)	0·847 (4)	−0·110 (6)	H(9*B*)*B*	0·893 (9)	0·661 (4)	0·255 (6)
H(10*A*)*A*	0·092 (9)	0·890 (4)	−0·116 (6)	H(10*A*)*B*	0·997 (9)	0·558 (4)	0·417 (6)
H(10*B*)*A*	0·289 (9)	0·931 (4)	−0·149 (6)	H(10*B*)*B*	0·927 (9)	0·540 (4)	0·285 (6)
H(11*A*)*A*	0·151 (9)	0·646 (4)	0·050 (6)	H(11*A*)*B*	0·696 (9)	0·811 (4)	0·293 (6)
H(11*B*)*A*	0·308 (9)	0·668 (4)	0·134 (6)	H(11*B*)*B*	0·844 (9)	0·773 (4)	0·227 (6)
H(12*A*)*A*	0·490 (9)	0·569 (4)	0·074 (6)	H(12*A*)*B*	1·051 (9)	0·882 (4)	0·299 (6)
H(12*B*)*A*	0·337 (9)	0·555 (4)	−0·011 (6)	H(12*B*)*B*	0·885 (9)	0·915 (4)	0·346 (6)
H(13*A*)*A*	0·355 (9)	0·480 (4)	0·132 (6)	H(13*A*)*B*	0·894 (9)	0·882 (4)	0·100 (6)
H(13*B*)*A*	0·177 (9)	0·525 (4)	0·108 (6)	H(13*B*)*B*	0·738 (9)	0·907 (4)	0·141 (6)
H(13*C*)*A*	0·333 (9)	0·542 (4)	0·215 (6)	H(13*C*)*B*	0·863 (9)	0·962 (4)	0·157 (6)
H(14*A*)*A*	0·399 (9)	0·630 (4)	−0·155 (6)	H(14*A*)*B*	0·668 (9)	0·808 (4)	0·491 (6)
H(14*B*)*A*	0·383 (9)	0·710 (4)	−0·205 (5)	H(14*B*)*B*	0·860 (9)	0·858 (4)	0·512 (6)
H(15*A*)*A*	0·063 (9)	0·695 (4)	−0·196 (5)	H(15*A*)*B*	0·955 (9)	0·774 (4)	0·638 (6)
H(15*B*)*A*	0·090 (9)	0·618 (4)	−0·127 (6)	H(15*B*)*B*	0·749 (9)	0·738 (4)	0·650 (6)
H(16*A*)*A*	0·012 (9)	0·604 (4)	−0·345 (6)	H(16*A*)*B*	0·656 (9)	0·835 (4)	0·729 (6)
H(16*B*)*A*	0·166 (9)	0·643 (4)	−0·375 (6)	H(16*B*)*B*	0·807 (9)	0·821 (4)	0·824 (6)
H(16*C*)*A*	0·209 (9)	0·556 (4)	−0·285 (6)	H(16*C*)*B*	0·799 (9)	0·876 (4)	0·714 (6)
H(N1)*A*	0·463 (9)	0·710 (4)	−0·006 (6)	H(N1)*B*	0·985 (9)	0·767 (4)	0·421 (6)
H(O1)*A*	0·182 (9)	1·097 (4)	−0·042 (6)	H(O1)*B*	0·813 (9)	0·379 (4)	0·432 (6)

hydrogen atoms were located, giving a conventional R value of 0·40. At this stage anisotropic temperature factors were introduced and after four more refinement cycles a difference map revealed the positions of all 52 H atoms. For the final refinement the temperature factors of the H atoms were locked at $B = 4·0$ Å^2, and all reflexions were given unit weight. The final R value was 0·052 for the 2081 observed reflexions. In the last cycle the average parameter shift expressed as a fraction of the e.s.d. was 0·7. The final atomic coordinates are given in Tables 1 and 2. The scattering factors were from *International Tables for X-ray Crystallography*

(1974). The computations were made on an IBM 370/165 computer using our own program system (Bergin, 1971). The stereo picture of the molecule (Fig. 3) was drawn by *ORTEP* (Johnson, 1965).*

The absolute configuration

Zymalkowski & Dornhege (1969) synthetized the basic aminotetralin skeleton from L-(+)-aspartic acid, showing that the absolute configuration of (−)-2-AT is *S* at asymmetric atom 2. In the present study their result was checked by applying the test suggested by Hamilton (1965) to the refined structure. The *R* values were 0·05263 and 0·05232 respectively for the (2*S*) and (2*R*) forms. The hypothesis that the (+)-2-AT studied here has a (2*R*) configuration is thus verified with a significance better than 0·005. This indicates that the active enantiomers of apomorphine and of the 2-aminotetralins have the same absolute configuration.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34784 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

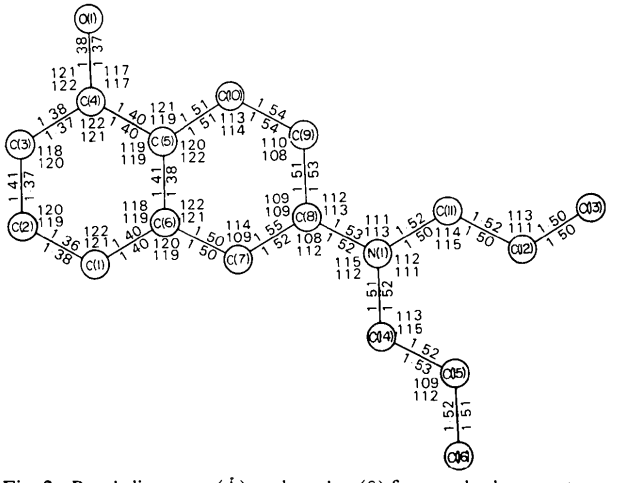

Fig. 2. Bond distances (Å) and angles (°) for non-hydrogen atoms in the aminotetralin molecule. The upper value refers to molecule *A*.

Table 3. *Least-squares planes of the aromatic rings in the two molecules*

Deviations of individual atoms are in Å. Asterisks mark atoms included in the calculations of the planes. E.s.d.'s in parentheses are in units of the last digit.

Molecule *A*: $0{\cdot}9700X - 0{\cdot}1598Y - 0{\cdot}1834Z = 1{\cdot}6806$
Molecule *B*: $-0{\cdot}2488X - 0{\cdot}1140Y + 0{\cdot}9618Z = -4{\cdot}7061$

	Molecule *A*	Molecule *B*
C(1)*	−0·002 (7)	−0·015 (7)
C(2)*	−0·006 (8)	0·011 (7)
C(3)*	0·015 (7)	0·000 (7)
C(4)*	−0·015 (7)	−0·007 (7)
C(5)*	0·006 (7)	0·003 (7)
C(6)*	0·002 (7)	0·008 (7)
C(7)	0·007 (7)	−0·016 (7)
C(10)	−0·014 (8)	−0·040 (7)
O(1)	−0·061 (6)	−0·062 (5)

Description of the structure

Geometry of the molecules

The standard chemical numbering of the atoms in the ring system of a 2-AT is shown in Fig. 1. The numbering system used below was chosen to facilitate comparison with dopaminergic substances studied earlier at this department. Values without parentheses in the text refer to molecule *A*, those in parentheses to molecule *B* of the unit cell. Values for bond distances and angles are given in Fig. 2; a full table can be obtained from the author. The mean standard deviations for bond lengths and angles involving non-hydrogen atoms only are 0·015 (0·014) Å and 1·2 (1·2)° respectively. The bond lengths to H atoms range from 0·88 (0·80) to 1·19 (1·17) Å, while the corresponding angles differ by up to 20 (18)° from the theoretical values.

The bond lengths and angles between non-hydrogen atoms nowhere deviate noticeably from what is ordinarily observed, and values for the two different molecules agree well.

The 2-AT molecule is quite flat with atoms C(1) through C(7), C(10), and O(1) approximately in one plane (*cf.* Table 3). When the (+) form is viewed as in Fig. 2, C(8) is behind and C(9) in front of this plane, and the non-aromatic ring thus assumes a half-chair conformation. (See also Fig. 3, where molecule *A* is depicted stereoscopically.) The N atom is attached equatorially, and the 2-AT molecule thus corresponds to the *trans* form of dopamine. The non-aromatic ring has some flexibility, indicated by the fact that in molecule *A* the N atom is 0·1 Å above the plane of the aromatic ring, while in molecule *B* it is 0·9 Å below. The torsion angles τ_1 [C(1)–C(6)–C(7)–C(8)] and τ_2 [C(6)–C(7)–C(8)–N(1)] also differ somewhat in the two molecules: τ_1 is 168 (151)° and τ_2 166 (−173)°. (The e.s.d. for all four angles is about 1·5°.)

The two propyl chains are fully extended from the N atom in both molecules. In molecule *A* one chain is approximately in the plane of the rings, while the plane of the other chain is perpendicular to the plane of the rings. In molecule *B* the planes of the propyl chains are perpendicular to the plane of the rings and to one another. This difference between the molecules is probably due to packing.

Table 4. *Hydrogen bonds*

The column labelled x',y',z' gives the symmetry code of acceptor atom Y'. The reference molecule is in x,y,z.

X	H	Y'	x',y',z'	$X\cdots Y'$	$H\cdots Y'$	$\angle X$–H$\cdots Y'$
O(1)*A*	H(O1)*A*	Cl*A*	$1-x, y-\frac{1}{2}, -z$	3·09 (1) Å	2·18 Å	169°
N(1)*A*	H(N1)*A*	Cl*A*	x,y,z	3·13 (1)	2·25	166
O(1)*B*	H(O1)*B*	Cl*B*	$1-x, y+\frac{1}{2}, 1-z$	3·10 (1)	2·15	169
N(1)*B*	H(N1)*B*	Cl*B*	$x-1, y, z$	3·09 (1)	2·27	160

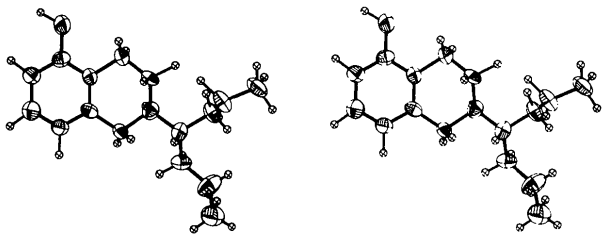

Fig. 3. Stereoscopic pair showing molecule *A*. Thermal ellipsoids for non-hydrogen atoms represent 50% probability. This figure shows the active (–) form.

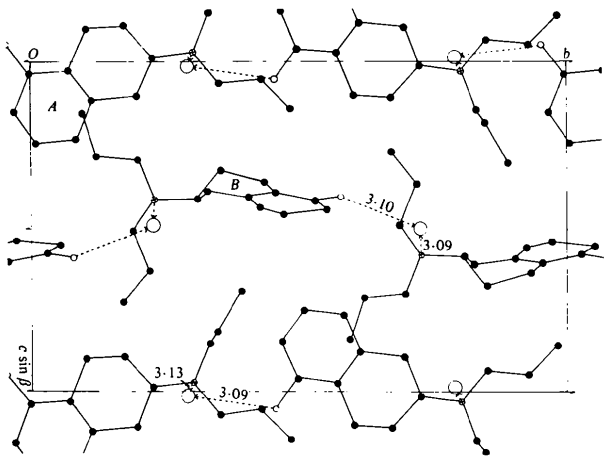

Fig. 4. Molecular packing. C, N and O atoms are represented by filled, crossed, and unfilled circles respectively. Chloride ions are larger unfilled circles. Broken lines represent hydrogen bonds (Å) with arrow-heads towards the acceptor atom.

Hydrogen bonds and molecular packing

The contents of one unit cell are shown in Fig. 4. The 2-AT molecules form infinite chains along the screw axes. In each chain the N atom of one molecule is connected *via* a Cl atom to the O atom of the next molecule by hydrogen bonds. Each chain consists of either *A* or *B* molecules and the chains are not interconnected. The four different hydrogen bonds thus formed all have lengths of about 3·1 Å, which is a normal value (see also Table 4). Apart from these hydrogen bonds there are no distances between non-hydrogen atoms shorter than 3·5 Å.

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