All the piperazine and hexahydropyrimidine rings of both isomers presently investigated adopt chair conformations. This may be proved by considering the torsion angles occurring in the rings.* The calculated asymmetry parameters (Duax & Norton, 1975) for these rings (*RING*; Párkányi, 1979) reveal small deviations [$(\Delta C_2)_{max} = 6{\cdot}6\,(5)°$, $(\Delta C_s)_{max} = 5{\cdot}0\,(5)°$] from the ideal chair conformation. This may be partly caused by the presence of N hetero-atoms in the rings. The deviations are larger in the case of *cis*-PTAP than in *trans*-PTAP. The presence of methyl and/or phenyl substituents at the hexahydropyrimidine rings in the above known structures seems neither to influence the chair distortions in some regular way nor to increase the calculated asymmetry parameters significantly.

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* See deposition footnote.

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The Structure of 4-(2-Chlorodibenz[*b*,*f*][1,4]oxazepin-11-yl)-1-methyl-1*H*$^+$-piperazinium Succinate Monohydrate (Loxapine Succinate Monohydrate)

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Abstract

The X-ray crystal structure of the psychoactive agent loxapine succinate monohydrate has been determined. $C_{18}H_{19}ClN_3O^+.C_4H_5O_4^-.H_2O$ is triclinic, space group $P\bar{1}$, with $a = 9{\cdot}702\,(3)$, $b = 14{\cdot}237\,(4)$, $c = 9{\cdot}436\,(4)$ Å, $\alpha = 92{\cdot}80\,(3)$, $\beta = 115{\cdot}82\,(3)$ and $\gamma = 76{\cdot}89\,(2)°$. The structure was solved by direct methods using *MULTAN* and refined by standard least-squares methods to $R = 0{\cdot}050$ for 2484 reflections with $I > 3\sigma(I)$. The central seven-membered heterocyclic ring is in a boat conformation while the piperazine ring is in the normal chair conformation. The dihedral angle between the planes of the benzene rings is 121°. There are two half-succinate molecules per asymmetric unit,

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each located on a center of symmetry. The distal N atom of the piperazine ring hydrogen bonds to one of the succinate O atoms, while the remaining three succinate O atoms hydrogen bond to the water molecule of crystallization.

Introduction

Loxapine succinate monohydrate is a psychoactive agent used in the treatment of schizophrenia. It is of interest to compare the protonated form of the molecule to the free base (Cosulich & Lovell, 1977; Petcher & Weber, 1976)* and to the known neurotransmitter dopamine.

Experimental

A sample of the free base was supplied by Lederle Laboratories and recrystallized from an aqueous solution containing a 1:1 mixture of loxapine and succinic acid. The density was measured by flotation: D_m = 1·333, D_x = 1·349 g cm^{-3}, for Z = 2. The crystals were clear rectangular plates and were found to be triclinic, space group $P\bar{1}$. The crystal used for data collection was of approximate dimensions 0·15 × 0·20 × 0·45 mm.

Unit-cell parameters (*Abstract*) were determined by the least-squares refinement of the first-moments of the 2θ values for 95 reflections in the range $10° < 2\theta < 50°$ (H. A. Levy, personal communication). Intensities were measured in the range $1° < 2\theta < 55°$, with the $\theta/2\theta$ scan method, on an Oak Ridge computer-controlled diffractometer using Nb-filtered Mo $K\bar{\alpha}$ radiation (λ = 0·71069 Å). The intensities of 4042 unique reflections were measured, 2484 of which were greater than $3\sigma(I)$. Extinction and absorption corrections (μ = 2·97 cm^{-1}) were not applied. All data were measured at 299 ± 1 K.

The structure was solved by direct methods using *MULTAN* (Germain, Main & Woolfson, 1971). All non-hydrogen atoms, including a water molecule of crystallization, were revealed. Full-matrix least-squares refinement with isotropic thermal parameters reduced the R value to 0·15. Further anisotropic full-matrix least-squares refinement reduced the R value to 0·09, at which point all H atoms, except those associated with O(6), the water molecule of crystallization, and the protonated succinate oxygen O(5), were located in a three-dimensional difference Fourier map. The difficulty in locating these H atoms was due to the positional disorder, denoted by the large thermal parameters, associated with the water molecule and succinate anion. The H atoms were placed into the refinement with isotropic thermal parameters and allowed to refine along with the non-hydrogen atoms. In the least-squares refinement each structure factor was weighted according to the equation $w(|F_o|)^{-1} = [\sigma^2(|F_o|) + 0{\cdot}0004|F_o^2|]$. The final measures of agreement are: $R(F)$ = 0·050, $R(F^2)$ = 0·065, $R_w(F)$ = 0·060 and σ = 1·767 {standard deviation of an observation of unit weight defined as $[\sum w|\Delta F|^2/(n-p)]$, where n is the number of observations and p the number of adjusted parameters}. The largest peak in the final difference Fourier map was 0·49 e Å^{-3} and associated with O(6). Final positional parameters for the non-hydrogen atoms are shown in Table 1.*

All refinement was performed with the XRAY system (Stewart, Kruger, Ammon, Dickinson & Hall,

* Only the results of Cosulich & Lovell will be considered due to the similarity of the determinations of the free base.

* Lists of structure factors, thermal parameters and hydrogen-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38076 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional positional parameters* (×10^4) *and equivalent isotropic temperature factors* (Å^2 ×10^4) *for the non-hydrogen atoms, with e.s.d.'s in parentheses*

	x	y	z	U†
C(1)	7894 (3)	433 (2)	765 (4)	418 (18)
C(2)	6529 (4)	1094 (3)	560 (4)	514 (21)
C(3)	6483 (5)	1706 (3)	1720 (5)	626 (25)
C(4)	7811 (4)	1676 (3)	3098 (5)	573 (22)
O(1)	10506 (3)	997 (2)	4749 (2)	482 (14)
C(5)	12140 (4)	2112 (2)	5183 (4)	536 (22)
C(6)	13369 (5)	2382 (3)	5069 (4)	588 (24)
C(7)	14120 (5)	1811 (3)	4275 (5)	601 (27)
C(8)	13683 (4)	975 (3)	3628 (4)	520 (22)
C(9)	11696 (4)	1284 (2)	4524 (4)	431 (18)
C(10)	12436 (4)	696 (2)	3716 (4)	425 (19)
C(11)	9184 (4)	1015 (2)	3331 (4)	435 (19)
C(12)	9248 (3)	367 (2)	2188 (4)	381 (17)
N(13)	12116 (3)	−195 (2)	3129 (3)	446 (16)
C(14)	10723 (3)	−352 (2)	2473 (3)	379 (18)
N(15)	10546 (3)	−1241 (2)	1845 (3)	405 (15)
C(16)	9350 (4)	−1716 (2)	1823 (4)	430 (19)
C(17)	8890 (4)	−2345 (2)	443 (4)	470 (20)
N(18)	10275 (3)	−3089 (2)	554 (3)	460 (17)
C(19)	11545 (4)	−2622 (2)	675 (4)	503 (21)
C(20)	11957 (4)	−1963 (2)	2014 (4)	474 (20)
C(21)	9870 (6)	−3744 (3)	−787 (5)	778 (30)
Cl‡	48536 (10)	11422 (9)	−12131 (13)	7440 (70)
O(2)	−1298 (2)	4124 (2)	6833 (4)	955 (22)
O(3)	1132 (4)	4042 (3)	7523 (4)	1100 (27)
C(22)	−220 (4)	4313 (2)	6611 (5)	534 (22)
C(23)	653 (4)	5134 (3)	4909 (5)	741 (27)
O(4)	4580 (5)	5468 (2)	2344 (5)	1179 (29)
O(5)	4473 (6)	3929 (3)	2074 (5)	1323 (36)
C(24)	4878 (5)	4568 (3)	4538 (6)	883 (32)
C(25)	4635 (5)	4702 (4)	2896 (7)	904 (34)
O(6)	4039 (6)	3997 (5)	9268 (6)	1766 (49)

† $U = \frac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.
‡ Values are ×10^5.

1972). The atomic scattering factors used were from Cromer & Mann (1968), except for H for which the factors of Stewart, Davidson & Simpson (1965) were used. The dispersion corrections of Cromer (1965) were used for chloride.

Discussion

An *ORTEP* drawing (Johnson, 1965) of the loxapine cation and half-succinate anions, including bond distances and angles, is shown in Fig. 1. The bond lengths and angles associated with the molecule are similar to those found in related compounds [clozapine and HUF-2046 (Petcher & Weber, 1976); amoxapine (Cosulich & Lovell, 1977)]. The most significant difference between the title compound (LS) and the free base (LFB) occurs at the site of protonation, N(18). There is an increase in the average bond length about N(18) [1·487 (4) Å, LS; 1·455 (4) Å, LFB].

The piperazine ring is in the normal chair conformation. The bond angles associated with the ring are essentially tetrahedral. The most noticeable deviation, however, occurs in the external angles about N(15). These angles are substantially larger than the internal angle, suggesting some electron delocalization into the N(15)–C(14) bond. The flattening at N(15), from an approximate tetrahedral configuration, is revealed when the deviations of N(15) and N(18) from the planes through C(14), C(16), C(20), and C(17), C(19) and C(21) are compared. The deviation for N(15) is 0·241 (3) Å while for N(18) it is −0·451 (3) Å (the four C atoms of the ring are coplanar within experimental error). The methyl group C(21) is attached equatorially at N(18). The conformation of the piperazine ring with respect to the oxazepine ring was

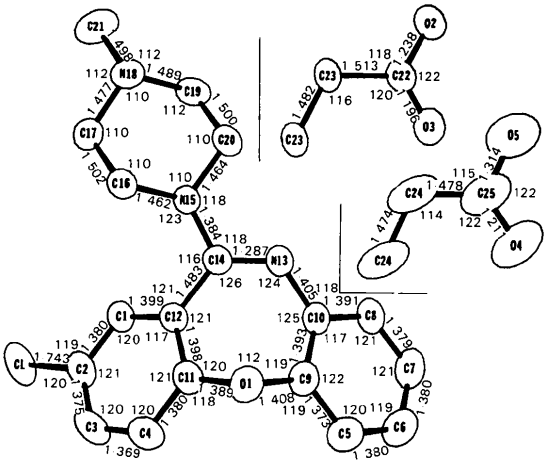


Fig. 1. Bond distances (Å) and bond angles (°) for loxapine succinate monohydrate. The non-hydrogen atoms are shown using 45% probability thermal ellipsoids. The average standard deviations in the bond lengths and bond angles are 0·005 Å and 0·3°, respectively.

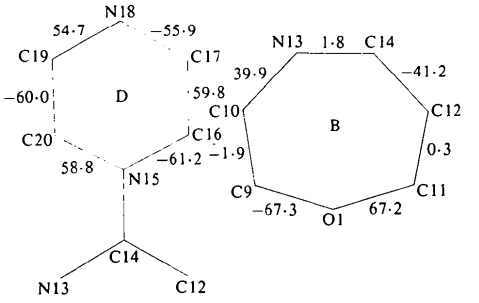
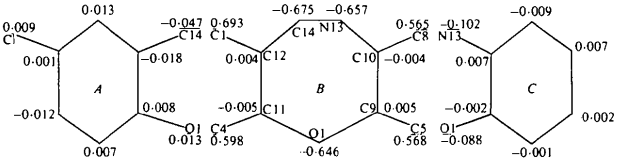


Fig. 2. Torsion angles (°) in the oxazepine and piperazine rings. The average standard deviation in the torsion angles is 0·4°. [α = N(13)–C(14)→N(15)–C(20) = 2·3°; β = N(13)–C(14)→N(15)–C(16) = 147·3°.]

analyzed by computing the torsion angles around the C(14)–N(15) bond. The torsion angle N(13)–C(14)–N(15)–C(20) is 2·3 (3)°, which is similar to the 1·2° found in the free base, indicating that these atoms are nearly coplanar. Torsion angles for the piperazine and oxazepine rings are shown in Fig. 2.

Bond lengths in the oxazepine ring show no unusual features when compared with individual values obtained from other structures (clozapine, LFB, amoxapine, and HUF-2046). In structures containing the −N=C< group, the bond length varies between 1·25 and 1·31 Å (Orioli, Lingafelter & Brown, 1964; Jensen & Jerslev, 1967; Cosulich & Lovell, 1977; Petcher & Weber, 1976). The distance found in the present structure is within this range and short enough to be considered a double bond in character. The C(14)–C(12) bond length is within the range of a pure C(sp^2)–C(sp^2) bond, 1·47–1·48 Å (Lide, 1962).

The overall geometry of the dibenzoxazepine ring system was studied by calculating least-squares planes through various sets of atoms. Details concerning these planes are shown in Fig. 3. The aromatic rings are



Ring *A*	C1 C2 C3 C4 C11 C12
Plane†	0·487*x* + 0·779*y* − 0·395*z* = 5·017
Ring *B*	C9 C10 C11 C12
	0·012*x* + 0·748*y* − 0·664*z* = 0·697
Ring *C*	C5 C6 C7 C8 C9 C10
	−0·300*x* + 0·421*y* − 0·856*z* = −4·270

† *x*,*y*,*z* are ångström coordinates referred to directions *a*,*b*,*c**.

Fig. 3. Least-squares planes in the dibenzoxazepine system. Deviations (Å) of the atoms from the planes are shown. The average standard deviation associated with the displacement of atoms from the least-squares planes is 0·004 Å.

planar within experimental error. N(13), O(1) and C(14) are slightly displaced from the aromatic rings *A* and *C*. The oxazepine ring *B* is in a boat conformation with C(9), C(10), C(11) and C(12) coplanar. N(13) and C(14) form the stern of the boat and are equally displaced from the plane [−0·657 (3), −0·675 (3) Å, respectively]. There is a pseudomirror plane bisecting the N(13)–C(14) bond and passing through O(1) (Fig. 2). The dibenzoxazepine system is folded so that the obtuse angle between the normals to the benzene rings is 121·4 (3)°. This is significantly larger than the angle found in the free base, 113·7°.

The anion in the crystal structure consists of a half-succinate molecule located on the center of symmetry $(0,\frac{1}{2},\frac{1}{2})$ and a second half-succinate molecule located on the center of symmetry $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. Based on bond lengths, O(5) appears to be protonated, although this H and those bound to the water molecule could not be located. O(2) is hydrogen bonded to the tertiary amine N(18) [N(18)–H(18) 0·89 (4), H(18)···O(2) 1·72 (4) Å; N(18)···O(2) 2·606 (3) Å; N(18)–H(18)···O(2) 177 (4)°]. The remaining succinate O atoms hydrogen bond to the water molecule [O(6)···O(3), 2·563 (6); O(6)···O(4), 2·653 (6); O(6)···O(5), 2·496 (6) Å], forming approximate tetrahedral angles about O(6) [O(5)--O(6)--O(4), 137·3 (3); O(4)--O(6)--O(3), 111·9 (2); O(3)--O(6)--O(5), 107·7 (2)°].

The packing and hydrogen bonding of the molecules are shown in Fig. 4. One succinate ion, composed of O(4), O(5), C(24) and C(25), forms chains running parallel to **c** with the succinate O atoms connected by symmetry-related water molecules. The second succinate ion hydrogen bonds directly to pairs of loxapine cations in addition to the water molecule.

In an effort to explore the similarities between the free base and the protonated form of the molecule, the free base was fit onto the protonated species using the program *BMFIT* (Nyburg, 1974). The r.m.s. deviation (Δ) in the position of the atoms is 0·16 Å.

It is interesting to explore the relationship of neuroleptic drugs to known neurotransmitters. For example, it has been shown that these drugs are capable of competing with dopamine (Fig. 5*a*) in synaptosomal preparations (Seeman, Chau-Wong, Tedesco & Wong, 1975; Burt, Enna, Creese & Snyder, 1975). One parameter which may be of importance for neuroleptic activity is the relationship of the protonated tertiary amino group to the aromatic ring system (Horn & Snyder, 1971). For the thioxanthenes (α-flupenthixol and α-chlorprothixene), tricyclic S-containing compounds, it appears that a conformationally asymmetric molecule is required for activity, in which the distances between the amino group and the two aromatic rings have average values of 6·03 and 7·45 Å (Horn, Post & Kennard, 1975). These values are very similar to the distances found for the loxapine cation and free base [6·11 (2) and 7·76 (2) Å, 6·19 (1) and 7·73 (2) Å, respectively] and also for several related dibenzodiazepines [5·93 (1) and 7·69 (1) Å, clozapine free base; 5·93 (2) and 7·87 (2) Å, clozapine dihydrobromide (Fillers & Hawkinson, 1982); and 5·94 (1) and 7·77 (1) Å for HUF-2046, a structural isomer of clozapine (Petcher & Weber, 1976)].

In an effort to discern which portion of the loxapine molecule may be responsible for its neuroleptic activity, the phenyl moiety and primary amine of dopamine.HCl (Bergin & Carlström, 1968) were superimposed onto both aromatic rings of the loxapine cation and the protonated amine N(18) (Fig. 5*b*) using the program *BMFIT* (Nyburg, 1974). During the fitting process, the centroids of each aromatic ring were matched exactly and the atoms of dopamine were allowed to refine; the weight of the N atom was taken to be six times that of a single C atom. The best fit was obtained using the aromatic ring *A* of loxapine (Fig. 5*c*) and the resulting distance between N atoms was 1·18 Å, which is similar to the 1·21 Å found in the free base and in several related compounds [clozapine free base and dihydrobromide, 0·99 and 0·92 Å respectively (Fillers & Hawkinson, 1982); HUF-2046, 0·96 Å (Petcher & Weber, 1976)].

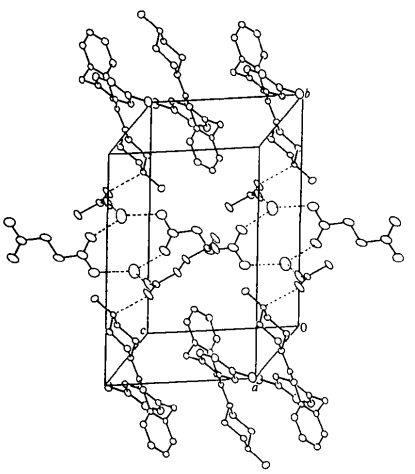
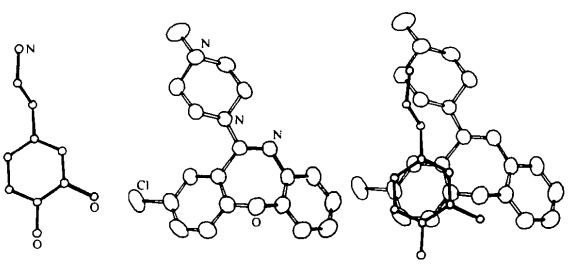


Fig. 4. Molecular packing and hydrogen bonding for loxapine succinate monohydrate viewed approximately along **a**. Hydrogen bonding is shown as dashed lines.



(*a*) (*b*) (*c*)

Fig. 5. (*a*) Dopamine and (*b*) loxapine molecule and (*c*) overlap of dopamine onto loxapine.

Another possibility of overlap exists between dopamine and a portion of the loxapine cation consisting of ring *C*, the hetero-atom bridge and N(15). Derivatives of clozapine, a closely related dibenzodiazepine featuring a 1,5-benzodiazepine portion, have been prepared and evaluated for neuroleptic activity (Ellefson, Woo, Miller & Kehr, 1978; Kukla, 1977). It was found, however, that the 1,5-benzodiazepine portion of the molecule (similar to the 1,5-benzoxazepine portion of loxapine) was not responsible for neuroleptic activity.

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4-Chloro-3-phenylfuroxan and 3-Chloro-4-phenylfuroxan*

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Abstract

Of the two isomers [$C_8H_5ClN_2O_2$, M_r = 196·50, $F(000)$ = 800], 4-chloro-3-phenylfuroxan (isomer *A*) has the lower melting point (339–340 K). It is orthorhombic, space group *Pbca*, with a = 17·156 (4), b = 12·803 (3), c = 7·835 (2) Å, U = 1720·9 (7) Å^3, Z = 8, D_x = 1·52 Mg m^{-3}, μ(Cu $K\alpha$) = 3·68 mm^{-1}. The higher-melting isomer (347–348 K, isomer *B*), 3-chloro-4-phenylfuroxan, is monoclinic, space group $P2_1/c$, with a = 14·011 (4), b = 9·713 (2), c = 14·198 (4) Å, β = 119·66 (2)°, U = 1679·0 (8) Å^3,

* Furoxan is furazan *N*-oxide.

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