approximately in the plane of the DHP ring. Steric considerations still require that the normals for the aryl and DHP rings be approximately perpendicular, however. The phenyl ring may adopt an orientation which puts the *ortho*-NO_2 substitutent either above or below the plane formed by C1–C2–C5. Since the DHP ring is neither flat nor symmetrically substituted these two orientations will be of different energies. The orientation observed is the one in which the NO_2 group is on the same side of the ring as the methyl group C8.

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Structure of *N*-(*N*-Isopropyl-*N*-propylaminoethyl)phenothiazine Hydrochloride

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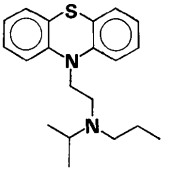
Abstract. $C_{20}H_{27}N_2S^+.Cl^-$, $M_r = 362{\cdot}9$, monoclinic, $P2_1/c$, $a = 12{\cdot}204\ (2)$, $b = 12{\cdot}032\ (2)$, $c = 13{\cdot}643\ (3)$ Å, $\beta = 103{\cdot}21\ (2)°$, $V = 1950{\cdot}4$ Å^3, $Z = 4$, $D_x = 1{\cdot}236$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}70930$ Å, $\mu = 3{\cdot}0$ cm^{-1}, $F(000) = 776$, $T = 100\ (2)$ K, final $R = 0{\cdot}051$ for 2469 reflections. The title compound crystallizes with a 'butterfly' fold angle of 134·7° between the two benzo rings. The N atom in the side chain is protonated and there is a hydrogen bond between it and the chloride ion. There are no unusual intramolecular distances or angles.

Introduction. Phenothiazine derivatives form a class of drugs which can be used as neuroleptics, sedatives, analgesics, anti-emetics and antihistamines. Although the pharmacological activity of the title compound has not been fully tested, the substituent bound to the phenothiazine skeleton causes this compound to be structurally similar to compounds that are known to possess anti-parkinsonian activity (diethazine and isothiazine) and antihistaminic activity (promethazine and thiazinamium methyl sulfate) (Tollenaere, Moereels & Raymaekers, 1979). In order better to understand the varied pharmacological activity of these compounds, we have been studying the structural characteristics of a series of phenothiazine derivatives (Klein, Conrad & Morris, 1985; Klein & Conrad, 1986; Southall, Malmstrom & Klein, 1987).



Experimental. Colorless crystal, approximate dimensions 0·30 × 0·25 × 0·40 mm recrystallized from a dichloromethane, hexane, 2-propanol (5:3:1) solution. Enraf–Nonius CAD-4 diffractometer with graphite-

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crystal-monochromatized Mo $K\alpha$ radiation. Unit-cell dimensions and systematic absences $h0l$, $l = 2n+1$ and $0k0$, $k = 2n+1$ uniquely determined the space group as $P2_1/c$. Unit-cell dimensions were determined by least-squares fit of 25 reflections with $36 \le 2\theta \le 47°$ measured on diffractometer. Three-dimensional intensity data collected in ω:2θ scan mode; total of 3643 independent reflections, 2469 observed with $I > 3\sigma(I)$; $1 \le 2\theta \le 50°$; $[(\sin\theta)/\lambda]_{max} = 0{\cdot}60$ Å^{-1}; $-14 \le h \le 14$, $0 \le k \le 14$, $0 \le l \le 16$. Data corrected for Lorentz and polarization effects. Three standard reflections measured every 2 h during data collection (400, 020, 004) showed no significant change in intensity. Absorption as a function of ψ was corrected empirically (maximum transmission 0·99, minimum transmission 0·90). Structure solved by direct methods using *MULTAN*11/82 series of programs (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). Initial E map contained all 24 non-hydrogen atoms. All H atoms were calculated on the basis of sp^2 or sp^3 geometry and a C—H bond length of 0·95 Å. Full-matrix least-squares refinement on F of 24 anisotropic non-hydrogen atoms (217 variables) with 27 H-atom positions and isotropic thermal parameters fixed. Final $R = 0{\cdot}051$, $wR = 0{\cdot}075$ where $w = 1/\sigma(F)^2$ and $\sigma(F)^2 = [\sigma(I)_{cs}{}^2 + (0{\cdot}04)^2(F^2)^2]$, $S = 2{\cdot}37$. In final least-squares cycle $(\Delta/\sigma)_{max} < 0{\cdot}1$. Maximum and minimum peaks in difference Fourier map were 0·97 and −0·43 e Å^{-3}, respectively. (The maximum peak in the difference map is not within reasonable bonding distance of any atoms in the structure.) Scattering factors, taken from *International Tables for X-ray Crystallography* (1974), are corrected for anomalous-scattering contributions. CAD-4 *SDP* programs used (Frenz, 1978).

Discussion. Final fractional coordinates for the non-hydrogen atoms are given in Table 1. The numbering system for the molecule can be found in Fig. 1. Bond lengths and angles have been deposited.* The title compound crystallizes as the HCl salt with one molecule in the asymmetric unit and the side-chain N(2) protonated. There is a hydrogen bond between N(2) and Cl [N(2)···Cl 3·040 (2) Å, N(2)—H···Cl 176·4 (1)°]. There are no unusual intramolecular distance or angles. A stereoscopic packing diagram can be found in Fig. 2.

The hybridization of the side-chain N atom appears to be characteristically sp^3 from its bond lengths and angles. However, N(1) (in the phenothiazine skeleton) appears to be hybridized between sp^2 and sp^3 resulting

*Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43958 (40 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Positional parameters and their estimated standard deviations*

Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as: $B_{eq} = \frac{4}{3}[a^2B_{1,1} + b^2B_{2,2} + c^2B_{3,3} + ab(\cos\gamma)B_{1,2} + ac(\cos\beta)B_{1,3} + bc(\cos\alpha)B_{2,3}]$.

	x	y	z	B_{eq}(Å^2)
Cl	0·52220 (8)	0·17702 (8)	0·89192 (6)	1·91 (2)
S	0·04787 (8)	0·23209 (9)	0·14026 (7)	2·12 (2)
N(1)	0·2531 (2)	0·1426 (2)	0·0919 (2)	1·44 (6)
N(2)	0·5610 (2)	0·1999 (3)	0·1192 (2)	1·49 (6)
C(1)	0·1054 (3)	0·2795 (3)	0·0409 (3)	1·61 (7)
C(2)	0·0540 (3)	0·3641 (3)	−0·0218 (3)	2·12 (8)
C(3)	0·1021 (4)	0·4028 (3)	−0·0975 (3)	2·32 (8)
C(4)	0·1986 (3)	0·3541 (3)	−0·1135 (3)	2·16 (8)
C(5)	0·2501 (3)	0·2679 (3)	−0·0526 (3)	1·69 (7)
C(6)	0·2043 (3)	0·2303 (3)	0·0261 (3)	1·49 (7)
C(7)	0·0761 (3)	0·0895 (3)	0·1296 (3)	1·78 (7)
C(8)	−0·0002 (3)	0·0094 (4)	0·1456 (3)	2·22 (8)
C(9)	0·0254 (3)	−0·1017 (4)	0·1433 (3)	2·46 (8)
C(10)	0·1254 (4)	−0·1332 (3)	0·1217 (3)	2·28 (8)
C(11)	0·2019 (3)	−0·0549 (3)	0·1034 (3)	1·90 (8)
C(12)	0·1780 (3)	0·0575 (3)	0·1087 (3)	1·50 (7)
C(13)	0·3700 (3)	0·1125 (3)	0·0957 (3)	1·57 (7)
C(14)	0·4458 (3)	0·2089 (3)	0·1401 (3)	1·50 (7)
C(15)	0·6191 (3)	0·0940 (3)	0·1579 (3)	2·10 (8)
C(16)	0·6498 (4)	0·0849 (4)	0·2711 (3)	3·6 (1)
C(17)	0·7208 (5)	−0·0190 (5)	0·3008 (4)	4·6 (1)
C(18)	0·6298 (3)	0·3048 (3)	0·1522 (3)	2·50 (8)
C(19)	0·5715 (5)	0·4051 (4)	0·0945 (4)	4·7 (1)
C(20)	0·7439 (4)	0·2948 (4)	0·1263 (4)	3·7 (1)

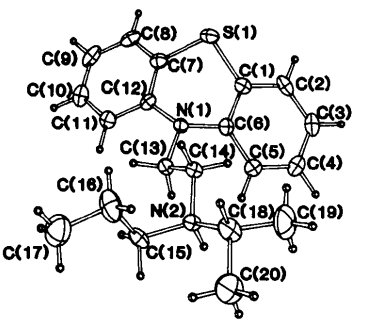

Fig. 1. Molecular structure and numbering system for one molecule of the title compound. The thermal ellipsoids are drawn at 50% probability levels.

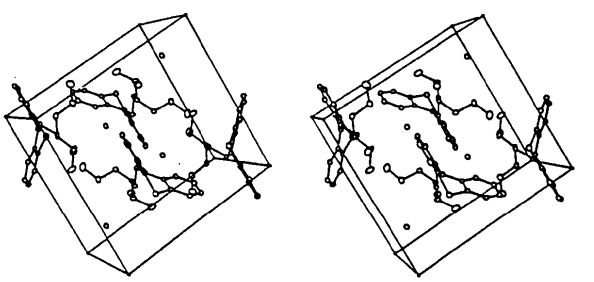

Fig. 2. Stereoscopic packing diagram of the contents of the unit cell looking down the a axis. The b axis is vertical and the c axis is horizontal.

in a flattened synperiplanar conformation. The average N(1)—C bond length, 1·438 (3) Å, is shorter than the average N(2)—C bond length, 1·507 (3) Å, and the average C—N(1)—C angle, 117·5 (2)°, is larger than the average C—N(2)—C angle, 112·7 (2)°. N(1) appears to be hybridized between sp^2 and sp^3 as a result of the competition between the stability that would be achieved by participation of the N(1) lone pair in the aromatic π system and the strain imposed on the hetero ring by the long S—C bonds which force the ring to exist in a boat conformation. This phenomenon has been observed in many neuroleptic drug molecules (Martin, Svensson, Bates & Ortega, 1985).

The angle between the benzo ring planes is 134·7° which compares favorably to the fold angle in other structurally similar compounds [*e.g.* promethazine, 141° (Marsau & Busetta, 1973); thiazinamium methyl sulfate, 136° (Marsau & Cam, 1973); diethazine, 136° (Marsau, 1971); isothiazine, 140° (Marsau & Calas, 1971) and 10-[di(*n*-propyl)aminoethyl]phenothiazine, 139·1° (Southall, Malmstrom & Klein, 1987)].

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Structure of 1-Acetoxy-1,2-dihydrothiazolo[3,2-*a*]quinolinium Perchlorate

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Abstract. $C_{13}H_{12}NO_2S^+.ClO_4^-$, $M_r = 345·8$, monoclinic, $P2_1/c$, $a = 11·108$ (5), $b = 8·236$ (4), $c = 15·723$ (4) Å, $\beta = 94·59$ (3)°, $V = 1433$ (2) Å^3, $Z = 4$, $D_x = 1·603$ g cm^{-3}, λ(Mo $K\bar{\alpha}$) = 0·71073 Å, $\mu = 4·3$ cm^{-1}, $F(000) = 712$, $T = 298$ K, $R = 0·051$ for 1996 observed reflections. The thiazolium ring is a distorted envelope, with bond lengths indicating delocalization through the N—C—S system. The ten atoms of the two fused six-membered rings are coplanar to within 0·015 Å. There is no possibility of hydrogen bonding, and stacking interactions of the aromatic fused ring systems dominate the packing motif.

Introduction. 1-Acetoxy-1,2-dihydrothiazolo[3,2-*a*]-quinolinium perchlorate (1*a*) was prepared as part of our continuing interest in the synthesis and biological activity of benzothiazolo[3,2-*a*]quinolinium salts (Cox, Jackson, Vargas, Baez, Colon, Gonzalez & de Leon, 1982; Cox, Jackson, Rivera & Ramirez, 1985). Preliminary biological studies (Ramirez, Morin, Cox & Escalona, 1984) on the effect of (1*b*) on muscular contraction were conducted using isolated frog skeletal muscle (*rectus abdominus*). The muscle response in the presence of (1) was compared with that of 10 n*M* acetylcholine (Ach). Experiments with the selective Ach blocker α-bungarotoxin indicate that (1*b*) effects a strong muscular contraction in the presence of this toxin. Therefore it is concluded that (1*b*) does not activate Ach receptors. In order to complete a structure–activity study of this series we had to prepare

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