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Prochlorperazine–Methanesulphonic Acid (1:2), a Phenothiazine Derivative

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Abstract. $C_{20}H_{24}ClN_3S.2CH_4O_3S$, 2-chloro-10-[3-(4-methyl-1-piperazinyl)propyl]phenothiazine–methanesulphonic acid (1:2), monoclinic, $C2/c$, a = 39·106 (2), b = 5·966 (2), c = 25·314 (2) Å, β = 115·73 (8)°, D_m = 1·423, D_c = 1·414 Mg m^{-3}, Z = 8; final R_w = 0·112. In the tricyclic group, C—S—C is 99·4 (9)°, C—S (mean) = 1·76 (2), C—N (mean) = 1·43 (2) and C—Cl = 1·55 (2) Å. The angle between the planes of the benzene rings is 136·1°. The piperazine ring has the chair conformation.

Introduction. The material was supplied by Maybaker. Colourless transparent needles were grown at a low temperature from a solution in *n*-propyl alcohol. The crystals tended to vaporize at room temperature. Systematic absences noted on Weissenberg photographs were hkl, $h + k \neq 2n$ and $h0l$, $l \neq 2n$, indicating space groups Cc or $C2/c$. Faint layer lines between the normal lines were observed in all oscillation films taken about **b**, but the corresponding Weissenberg photographs did not exhibit discrete reflexions. Intensities were collected on a Philips PW 1100 four-circle diffractometer with graphite-monochromated Mo $K\alpha$ (λ = 0·7107 Å) radiation at 293 K. The ω-scan mode was used with a scan rate of 0·033° s^{-1} and a scan width of 1·0° in θ. Background counts of 15 s on each side of the reflexion were taken. 2785 reflexions, including 315 systematically extinct and 825 rated as unobserved [$I < 1{\cdot}65\sigma(I)$], were measured within a sphere θ_{max} = 20°. The lattice constants were obtained by least squares from the 2θ, χ and φ angles for 25 reflexions. Only Lorentz–polarization corrections were applied as μr for the crystal (0·15 × 0·3 × 0·6 mm) was <0·15.

Analysis of the $|E|$ statistics and distribution indicated the space group $C2/c$. With *SHELX* 76 (Sheldrick, 1976), which incorporates a multi-solution tangent-formula phasing procedure, five reflexions were hand-selected from 442 with $E_{min} \geq 1{\cdot}2$. 31 of the non-H atoms were located from the E map with the highest figure of merit. In addition, a strong peak was indicated 1·7 Å from C(10); this peak, designated Cl(2), was apparent in all subsequent Fourier syntheses and had to be accounted for. The first Fourier map located the remaining four non-H atoms, and full-matrix least-squares refinement of coordinates and individual isotropic B's of non-H atoms brought R to 0·294. The programs used were from *SHELX* 76 and the XRAY system (1976); $R = \sum||F_o| - |F_c||/\sum|F_o|$; the function minimized, $R_w = \sum w(hkl)[|F_o(hkl) - F_c(hkl)|]^2$, where $w(hkl)$ = the weighting factor. Scattering factors of Cromer & Mann (1968) were used for Cl, S, O, N and C, and those of Stewart, Davidson & Simpson (1965) for H.

Most of the H atoms were found on a difference synthesis, but futher refinement with all 67 atoms did not reduce R substantially. However, when Cl(2) was included, and Cl(1) and Cl(2) were each assigned site-occupation factors of 0·5, six cycles with anisotropic β's of non-H atoms converged to a final R for 2470 reflexions of 0·115 [R_w = 0·112, with $w(hkl) = \sin\theta/A \times C/F_o$ with A = 0·23 and C = 40·0]. When allowed to refine freely, the H atoms of the methyl groups tended to drift; therefore, with the exception of the H atoms of the tricyclic group, the remaining H atoms were placed in idealized positions and constrained to ride on the C or O atoms to which they were attached; they were assigned isotropic thermal parameters derived from those of the carrier atoms. The site-occupancy factors of Cl(1) and Cl(2) refined to 0·53 and 0·49 respectively.

The presence of the two half-Cl atoms was not considered satisfactory and several trials were carried out on the assumption that some regular arrangement of

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Table 1. *Final atomic fractional coordinates* ($\times 10^4$, *for* H $\times 10^3$) *with e.s.d.'s in parentheses*

	x	y	z
Cl(1)	1513(2)	5252(16)	9824(3)
Cl(2)	3105(2)	4675(17)	7856(4)
S(1)	2350(2)	-1251(8)	8945(2)
C(1)	1751(4)	3747(35)	9583(7)
C(2)	1924(6)	1876(41)	9926(9)
C(3)	2108(6)	404(35)	9740(7)
C(4)	2124(4)	712(28)	9210(6)
C(5)	1959(4)	2601(29)	8860(6)
C(6)	1780(4)	4171(33)	9062(7)
N(1)	1993(3)	2911(22)	8329(5)
C(7)	2566(5)	591(29)	8645(7)
C(8)	2912(5)	105(40)	8674(8)
C(9)	3080(6)	1513(51)	8430(8)
C(10)	2891(5)	3412(55)	8136(8)
C(11)	2533(5)	3995(35)	8115(7)
C(12)	2365(4)	2554(28)	8361(7)
C(13)	1743(5)	4451(31)	7889(7)
C(14)	1325(4)	3733(28)	7625(7)
C(15)	1098(5)	5262(38)	7142(8)
N(2)	691(3)	4899(20)	6835(5)
C(16)	481(5)	6341(31)	6329(6)
C(17)	90(7)	5819(81)	5996(20)
N(3)	-116(3)	4406(25)	6129(5)
C(18)	85(5)	3041(30)	6650(6)
C(19)	477(6)	3455(50)	6985(9)
C(20)	-504(6)	3758(46)	5764(11)
S(2)	920	1664(10)	5667
O(1)	545(4)	1407(32)	5179(7)
O(2)	928(6)	898(29)	6217(7)
O(3)	1051(5)	3891(22)	5721(7)
C(21)	1212(7)	-131(45)	5500(11)
S(3)	680(2)	8180(10)	8216(4)
O(4)	399(4)	8667(30)	8431(10)
O(5)	769(4)	5837(22)	8268(7)
O(6)	580(5)	8995(26)	7653(8)
C(22)	1089(7)	9602(45)	8669(13)

	x	y	z
H(1)	159	494	972
H(2)	191	161	1034
H(3)	225	-103	1001
H(6)	167	569	882
H(8)	306	-141	889
H(9)	336	114	847
H(10)	302	446	792
H(11)	239	554	791
H(131)	177	608	809
H(132)	183	456	754
H(141)	122	380	796
H(142)	130	204	746
H(151)	121	516	682
H(152)	114	694	732
H(161)	62	624	604
H(162)	50	804	649
H(171)	7	524	558
H(172)	-6	741	594
H(181)	-5	329	694
H(182)	5	131	651
H(191)	50	403	741
H(192)	61	184	703
H(201)	-68	522	566
H(202)	-60	256	600
H(203)	-52	301	536
H(211)	150	-6	585
H(212)	111	-182	546
H(213)	121	38	509
H(214)	36	252	528
H(221)	118	905	912
H(222)	131	926	853
H(223)	103	1138	864
H(224)	15	776	814

the two molecules, one containing Cl(1) and the other Cl(2), could be discovered. The faint interlayer lines on the oscillation and Weissenberg photographs suggested a cell doubled on b containing eight molecules of each type; however, refinements on this basis failed to converge. The possibility of the noncentrosymmetric space group Cc with one molecule of each type forming the asymmetric unit was investigated, but R remained at 0·236 and bond lengths and angles were unsatisfactory. Thus we conclude that a specific type of disorder exists in which the two enantiomorphs must be present in almost equal numbers, but in random arrangement; possibly the crystal is composed of domains, each containing one of the individual types. Energy calculations, in progress in this laboratory, should show that both configurations must be at or near the global energy minimum.

The final positional parameters are given in Table 1.*

Discussion. Prochlorperazine has actions and uses similar to those of chlorpromazine but is a more potent tranquillizer and has powerful anti-emetic properties (*Martindale: The Extra Pharmacopoeia*, 1977). Bond lengths and angles are listed in Table 2; molecular configuration and atomic numbering are illustrated in Fig. 1 (Johnson, 1970). Although the C–C lengths within the benzene rings show rather large deviations, the average values [1·386 Å in C(1)–C(6) and 1·388 Å in C(7)–C(12)] are close to accepted values. Within the central ring system, the mean C–S 1·757 (19), mean C–N 1·428 (22) Å, C–S–C 99·4 (9), and C–N–C 115·9 (11)°, are in good agreement with those found in related compounds (Chu & van der Helm, 1975). The two C–Cl bonds are exceptionally short; however, in view of the disorder, too much weight cannot be attached to these values. For example, refinements carried out on the molecule with Cl(1) or Cl(2) alone gave 1·70 and 1·73 Å respectively. The sum of the angles around N(1) is 354·5°; N(1) is thus at the apex of a flattened pyramid with C(5), C(12), C(13) as the base. In the methanesulphonic acid groups, S–O lengths are within the accepted ranges (*International Tables for X-ray Crystallography*, 1962), while the

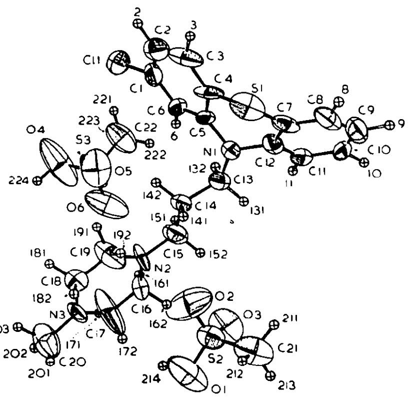

Fig. 1. Thermal-vibration ellipsoids and atomic numbering. ⊕ denotes H atoms.

Table 2. *Bond lengths* (Å) *and angles* (°)

C(1)–C(2)	1.395(29)	N(1)–C(13)	1.447(19)
C(2)–C(3)	1.344(34)	C(13)–C(14)	1.537(22)
C(3)–C(4)	1.381(28)	C(14)–C(15)	1.473(24)
C(4)–C(5)	1.405(22)	C(15)–N(2)	1.452(19)
C(5)–C(6)	1.393(28)		
C(6)–C(1)	1.395(28)	N(2)–C(16)	1.463(20)
C(1)–Cl(1)	1.592(23)	C(16)–C(17)	1.424(32)
		C(17)–N(3)	1.307(48)
		N(3)–C(18)	1.456(21)
C(7)–C(8)	1.357(29)	C(18)–C(19)	1.415(27)
C(8)–C(9)	1.365(37)	C(19)–N(2)	1.365(32)
C(9)–C(10)	1.380(39)	N(3)–C(20)	1.445(22)
C(10)–C(11)	1.424(31)		
C(11)–C(12)	1.382(28)	S(2)–O(1)	1.458(13)
C(12)–C(7)	1.418(22)	S(2)–O(2)	1.451(20)
C(10)–Cl(2)	1.513(29)	S(2)–O(3)	1.409(15)
		S(2)–C(21)	1.748(31)
C(4)–S(1)	1.768(19)	S(3)–O(4)	1.451(24)
C(7)–S(1)	1.746(20)	S(3)–O(5)	1.433(14)
C(5)–N(1)	1.419(23)	S(3)–O(6)	1.392(21)
C(12)–N(1)	1.437(21)	S(3)–C(22)	1.732(24)
C(6)–C(1)–C(2)	121.1(19)	C(3)–C(4)–S(1)	121.5(13)
C(1)–C(2)–C(3)	119.6(21)	C(8)–C(7)–S(1)	120.0(15)
C(2)–C(3)–C(4)	120.7(18)	C(6)–C(5)–N(1)	121.9(15)
C(3)–C(4)–C(5)	121.1(18)	C(11)–C(12)–N(1)	123.2(14)
C(4)–C(5)–C(6)	118.3(17)	C(5)–N(1)–C(13)	120.1(14)
C(5)–C(6)–C(1)	119.0(17)	C(12)–N(1)–C(13)	117.8(14)
Cl(1)–C(1)–C(2)	114.8(17)		
Cl(1)–C(1)–C(6)	124.1(15)		
		N(1)–C(13)–C(14)	113.2(15)
C(12)–C(7)–C(8)	121.6(18)	C(13)–C(14)–C(15)	109.4(15)
C(7)–C(8)–C(9)	120.5(21)	C(14)–C(15)–N(2)	118.5(17)
C(8)–C(9)–C(10)	120.1(23)	C(15)–N(2)–C(16)	116.7(15)
C(9)–C(10)–C(11)	120.4(24)	C(15)–N(2)–C(19)	127.3(14)
C(10)–C(11)–C(12)	118.9(19)		
C(11)–C(12)–C(7)	118.4(16)		
Cl(2)–C(10)–C(9)	112.8(19)	C(19)–N(2)–C(16)	115.9(14)
Cl(2)–C(10)–C(11)	126.8(22)	N(2)–C(16)–C(17)	116.1(25)
		C(16)–C(17)–N(3)	127.7(34)
C(4)–S(1)–C(7)	99.4(9)	C(17)–N(3)–C(18)	116.4(18)
S(1)–C(7)–C(12)	118.4(14)	N(3)–C(18)–C(19)	117.6(19)
C(7)–C(12)–N(1)	118.3(16)	C(18)–C(19)–N(2)	125.4(19)
C(12)–N(1)–C(5)	115.9(11)		
N(1)–C(5)–C(4)	119.7(16)	C(17)–N(3)–C(20)	126.9(21)
C(5)–C(4)–S(1)	117.4(14)	C(18)–N(3)–C(20)	115.7(17)
O(1)–S(2)–C(21)	104.7(11)	O(4)–S(3)–C(22)	106.6(14)
O(2)–S(2)–C(21)	107.1(13)	O(5)–S(3)–C(22)	107.4(10)
O(3)–S(2)–C(21)	110.6(12)	O(6)–S(3)–C(22)	105.9(13)
O(1)–S(2)–O(2)	112.0(11)	O(4)–S(3)–O(5)	110.8(12)
O(2)–S(2)–O(3)	110.4(10)	O(5)–S(3)–O(6)	112.5(12)
O(3)–S(2)–O(1)	111.8(10)	O(6)–S(3)–O(4)	113.2(12)

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* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34538 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

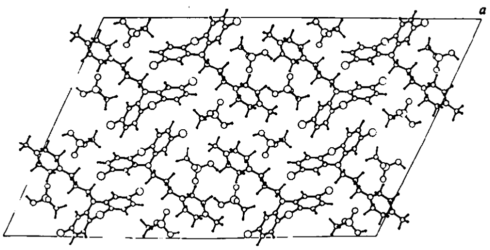

Fig. 2. The structure viewed down **b**.

Table 3. *Mean-plane parameters and deviations* (Å) *of atoms from the plane*

E.s.d.'s of deviations range from 0·02 to 0·03 Å.

Deviations of atoms defining the plane		Distances of atoms not defining the plane	
(I) C(1)-C(6)			
$28.0005x + 3.0230y + 3.0821z = 9.0117$			
C(1)	-0.0226	S(1)	-0.0529
C(2)	0.0019	N(1)	0.0158
C(3)	0.0148	C(13)	-0.3543
C(4)	-0.0146	Cl(1)	-0.1598
C(5)	-0.0098		
C(6)	0.0262		
(II) C(7)-C(12)			
$2.7993x + 3.0171y + 18.8189z = 17.1702$			
C(7)	-0.0049	S(1)	-0.0563
C(8)	0.0002	N(1)	-0.0597
C(9)	0.0128	C(13)	-0.4931
C(10)	-0.0204	Cl(2)	-0.1125
C(11)	0.0155		
C(12)	-0.0031		
(III) N(2)-C(16)-C(17)-N(3)-C(18)-C(19)			
$-18.6336x + 4.1113y + 17.6865z = 12.8593$			
N(2)	-0.0441	C(15)	-0.1102
C(16)	0.0452	C(20)	-0.1807
C(17)	-0.0298		
N(3)	0.0083		
C(18)	-0.0059		
C(19)	0.0263		

S–C lengths (mean 1·70 Å) show partial double-bond character.

Table 3 shows that the benzene rings are planar, with S(1) and N(1) slightly displaced from the planes. The dihedral angle is 136·1°, which agrees well with values found in other phenothiazine derivatives (McDowell, 1976). If the torsion angles τ_1 to τ_8 in Table 4 are compared with those of chlorpromazine (McDowell, 1977), it is found that although the upper part of the tail bears a close resemblance to that of chlorpromazine the lower part is far more extended. The packing of the molecules is shown in Fig. 2. The shortest N–O distances [N(2)–O(2) = 3·18, N(2)–O(6) = 3·33, N(3)–O′(4) = 3·30 Å] indicate that the expected formation of hydrogen bonds between N(2), N(3) and the hydroxyl groups constitutes at most a very weak system. Also, the lack of definition in the locations of H(214) and H(224) makes interpretation difficult. The configurations of the two different molecules are illustrated in Fig. 3. A crystal of prochlorperazine, therefore, is composed of *four* molecular species: the two types shown, plus their mirror images. This situation is

Table 4. *Selected torsion angles* (°)

E.s.d.'s are about 1·5°.

τ_1	C(4)-C(5)-N(1)-C(13)	162.7	τ_9	C(15)-N(2)-C(16)-C(17)	173.7
τ_2	C(7)-C(12)-N(1)-C(13)	-160.2	τ_{10}	C(15)-N(2)-C(19)-C(18)	-175.3
τ_3	C(5)-N(1)-C(13)-C(14)	-64.5	τ_{11}	C(19)-N(2)-C(16)-C(17)	-10.1
τ_4	C(12)-N(1)-C(13)-C(14)	144.3	τ_{12}	C(16)-N(2)-C(19)-C(18)	9.0
τ_5	N(1)-C(13)-C(14)-C(15)	-174.3	τ_{13}	N(2)-C(16)-C(17)-N(3)	9.9
τ_6	C(13)-C(14)-C(15)-N(2)	-179.1	τ_{14}	N(2)-C(19)-C(18)-N(3)	-5.9
τ_7	C(14)-C(15)-N(2)-C(16)	-175.3	τ_{15}	C(16)-C(17)-N(3)-C(20)	-174.4
τ_8	C(14)-C(15)-N(2)-C(19)	9.1	τ_{16}	C(19)-C(18)-N(3)-C(20)	173.2
			τ_{17}	C(16)-C(17)-N(3)-C(18)	-6.6
			τ_{18}	C(19)-C(18)-N(3)-C(17)	3.9

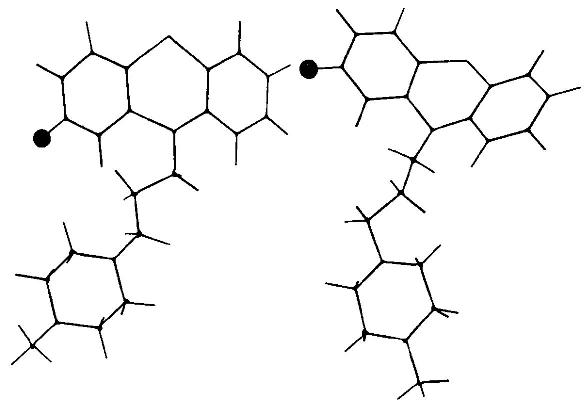

Fig. 3. Molecular models showing the topographies of the two enantiomorphs.

not unusual; comparable results were found in triflupromazine (Phelps & Cordes, 1974), dihydroanthracene III (Chu & Chung, 1976) and *n*-isopropylphenothiazine (Chu & van der Helm, 1976).

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A New Cardenolide: 5β-Hydroxygitoxigenin†

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Abstract. $C_{23}H_{34}O_6$, orthorhombic, $P2_12_12_1$, a = 11·290 (2), b = 24·638 (2), c = 7·122 (4) Å, V = 1981·1 Å^3, Z = 4, D_x = 1·363, D_m = 1·358 Mg m^{-3}. The structure was refined to R = 0·030 for 1847 observed reflexions. Its stereochemistry is similar to that of digitoxigenin, with the two terminal rings *cis* fused to the two central rings. The five-membered ring *D* assumes the α-envelope conformation at C(15). The X-ray analysis confirms the molecular formula and stereochemistry as determined by chemical and spectroscopic methods. There are two inter- and two intramolecular O—H···O bonds.

Introduction. New cardenolides are currently being prepared by chemical and microbiological methods in a search for active but less toxic compounds. A viable alternative method involves bioconversion by the use of plant cell suspension cultures. Recently, 5β-hydroxygitoxigenin has been isolated by I. A. Veliky and A. Jones at the National Research Council of Canada from cultures of *Daucus carota* Ca68 incubated with gitoxigenin. The compound has been identified and its chemical formula assigned on the basis of infrared, NMR and mass spectra. The present X-ray analysis was undertaken to establish the stereochemistry of this novel compound with OH substituents at C(3), C(5), C(14) and C(16). A summary of the biochemical and crystallographic results has been reported by Veliky, Jones, Przybylska & Ahmed (1979).

Colourless prismatic crystals, m.p. 507–509 K (with decomposition), were obtained by evaporation of a solution in ethanol and water and had to be grown to an appreciable length (>2 mm) to get a specimen of satisfactory thickness. A fragment 0·17 × 0·23 × 0·30 mm was mounted along c^* which is the prism axis. The space group was established from precession films, and the data were measured on a Picker four-circle automatic diffractometer with Ni-filtered Cu radiation [$\lambda(K\alpha_1)$ = 1·54050, $\lambda(K\alpha_2)$ = 1·54434 Å]. The cell parameters were derived from the angular settings of eight reflexions (2θ = 66 to 110°) and their equivalents.

Table 1. *Fractional coordinates* (×10^4) *for non-hydrogen atoms and* B_{eq} (Å^2) (= *average of three principal axes of the thermal ellipsoids*)

	x	y	z	B_{eq}
O(1)	7174 (2)	5019 (1)	3139 (3)	5·02
O(2)	9025 (2)	5305 (1)	2940 (3)	5·35
O(3)	6024 (1)	−9 (1)	2079 (3)	4·20
O(4)	8296 (1)	358 (0)	1701 (2)	3·00
O(5)	9256 (1)	2882 (1)	257 (2)	2·79
O(6)	7982 (2)	3703 (1)	−1365 (2)	3·45
C(1)	6836 (2)	949 (1)	4414 (3)	2·74
C(2)	5634 (2)	869 (1)	3482 (4)	3·17
C(3)	5748 (2)	543 (1)	1692 (4)	3·23
C(4)	6651 (2)	802 (1)	382 (3)	2·70
C(5)	7861 (2)	898 (1)	1287 (3)	2·21
C(6)	8707 (2)	1169 (1)	−92 (3)	2·68
C(7)	8427 (2)	1767 (1)	−449 (3)	2·51
C(8)	8313 (2)	2095 (1)	1362 (3)	2·07
C(9)	7402 (2)	1827 (1)	2672 (3)	1·97
C(10)	7763 (2)	1229 (1)	3151 (3)	2·21
C(11)	7166 (2)	2174 (1)	4410 (3)	2·75
C(12)	6777 (2)	2739 (1)	3811 (3)	2·46
C(13)	7723 (2)	3050 (1)	2667 (3)	2·13
C(14)	8114 (2)	2702 (1)	941 (3)	1·95
C(15)	7179 (2)	2839 (1)	−536 (3)	2·46
C(16)	7028 (2)	3452 (1)	−379 (3)	2·68
C(17)	7062 (2)	3554 (1)	1779 (3)	2·28
C(18)	8761 (2)	3189 (1)	3953 (4)	3·11
C(19)	8943 (2)	1213 (1)	4232 (4)	3·00
C(20)	7441 (2)	4117 (1)	2286 (3)	2·30
C(21)	6536 (2)	4519 (1)	2873 (5)	4·39
C(22)	8478 (2)	4371 (1)	2275 (4)	3·06
C(23)	8327 (2)	4932 (1)	2792 (4)	3·49

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