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Structures of Two 5-Hydroxytryptamine Receptor Agonists

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Abstract. 8-Methoxy-2-(*n*-propylamino)tetralin (8MeO-PAT) hydrochloride, $C_{14}H_{22}NO^+.Cl^-$, M_r = 255.8, monoclinic, $P2_1/n$, a = 9.2229 (4), b = 8.8051 (6), c = 17.6475 (7) Å, β = 93.513 (50)°, V = 1430.4 Å^3, Z = 4, D_x = 1.188 g cm^{-3}, λ(Cu $K\alpha$) = 1.54184 Å, μ = 22.59 cm^{-1}, $F(000)$ = 552, T = 298 K, final R = 0.0542 with 1722 independent data. 2-(Di-*n*-propylamino)-8-hydroxytetralin (8OH-DPAT) hydrochloride, $C_{16}H_{26}NO^+.Cl^-$, M_r = 283.8, monoclinic, $P2_1/n$, a = 9.9587 (7), b = 13.5746 (6), c = 12.1558 (6) Å, β = 94.537 (6)°, V = 1638.1 Å^3, Z = 4, D_x = 1.151 g cm^{-3}, λ(Cu $K\alpha$) = 1.54184 Å, μ = 19.00 cm^{-1}, $F(000)$ = 616, T = 298 K, final R = 0.1781 with 1550 independent data. The structure solution of 8OH-DPAT was hindered by the poor quality of the one crystal obtained. 8MeO-PAT and 8OH-DPAT are agonists of the 5-hydroxytryptamine (5-HT) receptor. When the aromatic rings of the two structures are superimposed, the propyl arm of 8MeO-PAT lies in the same position as the C(11) to C(13) arm of 8OH-DPAT. However, the torsion angles at N(1)—C(11) show a 20° deviation. 8OH-DPAT packs in an infinite stack with pairs of molecules related by an inversion centre. The Cl ion in 8MeO-PAT forms salt bridges that influence molecular packing. Adjacent molecules are rotated through 180° in the same plane.

Introduction. Knowledge of the conformations of neurotransmitters, peptide hormones and drugs is a prerequisite in understanding their mode of action. Such structures provide a starting point in the design of new agonists (a ligand binding tightly to a receptor and promoting the desired response) or antagonists (a ligand blocking the desired response), since the three-dimensional structures of the receptors for the most part remain elusive.

8-Methoxy-2-(*n*-propylamino)tetralin (8MeO-PAT) is an analogue of 2-(di-*n*-propylamino)-8-hydroxytetralin (8OH-DPAT) which is an agonist acting

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selectively at the 5-HT_{1A} receptor subtype (Fig. 1). This receptor is believed to be involved in physiological functions, such as thermoregulation, adenylate cyclase modulation and blood pressure, in the central nervous system (Peroutka, 1988).

Experimental. Crystals of 8MeO-PAT and 8OH-DPAT were grown by isothermal distillation of ether into methanol solutions. Laminar crystals of each were characterized by Weissenberg photography. Only one crystal of 8OH-DPAT was available. The data sets were collected on a Stoë STADI-4 diffractometer using graphite-monochromated Cu $K\alpha$ radiation.

The orientation matrix used for 8MeO-PAT data collection was derived from 11 reflections with $30 < 2\theta < 35°$, and accurate unit-cell dimensions were determined using 24 reflections measured at $\pm\omega$ in a $30 < 2\theta < 32°$ scan range. The orientation matrix used for 8OH-DPAT data collection was derived from eight reflections with $31 < 2\theta < 34°$, whilst accurate unit-cell dimensions were determined using 33 reflections measured at $\pm\omega$ in the same 2θ scan range.

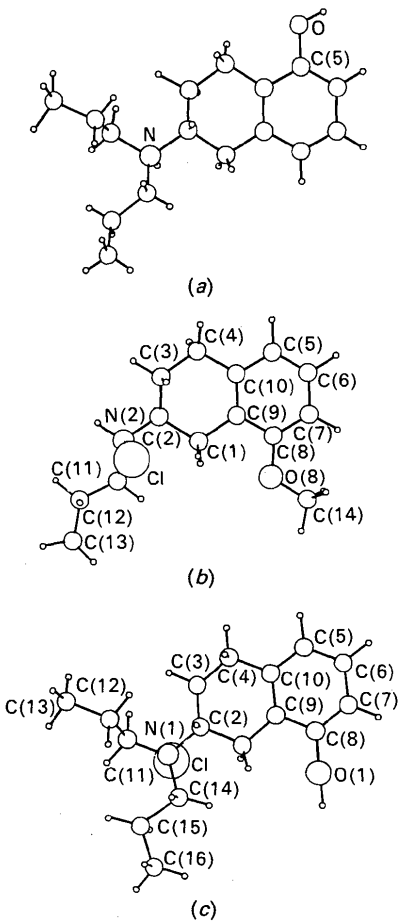

Fig. 1. Numbering scheme for atoms in (*a*) 5OH-DPAT, (*b*) 8MeO-PAT and (*c*) 8OH-DPAT.

Table 1. *Experimental data*

		8MeO-PAT	8OH-DPAT
Crystal dimensions (mm)		0.13 × 0.50 × 0.38	0.43 × 0.18 × 0.33
Reflections to determine lattice parameters		24	33
Max. $\sin\theta/\lambda$ ($Å^{-1}$)		0.5617	0.5567
Scan technique		$\omega/2\theta$	$\omega/2\theta$
hkl range	h	−10,10	−11,11
	k	0,9	0,11
	l	0,19	0,13
Standard reflections		$\bar{1}30$, $\bar{1}16$, 116	$\bar{2}04$, $\bar{3}21$, 124
Total data measured		2182	2142
Data used in refinement [$F > 6\sigma(F)$]		1722	1550
Parameters refined		180	144
R		0.0542	0.1781
wR		0.0670	—
S		1.288	2.852
Weighting scheme parameter x in $w^{-1} = \sigma^2(F) + xF^2$		0.004646	—
Max. Δ/σ, last cycle		0.144	1.654
Final difference map (e $Å^{-3}$)	max.	0.399	0.882
	min.	−0.260	−0.637

In both cases three intensity control reflections were measured every 2 h and no significant variation in intensity occurred during data collection. However, the peak shapes for the 8OH-DPAT crystal were unsatisfactory and therefore a damaged crystal was suspected. All the observed [$I > 3\sigma(I)$] reflection intensities were corrected for Lorentz and polarization effects but not for absorption or extinction.

A trial position for the Cl atom of 8MeO-PAT was found from a Patterson synthesis using *SHELX*76 (Sheldrick, 1976). In the resulting difference Fourier map all non-H atoms except those of the propylamino group were located. This part of the molecule was identified in subsequent difference Fourier maps. Non-H atoms were refined anisotropically (on F), with H atoms, which were added in their calculated positions, allowed to ride on the atoms to which they were attached. The isotropic temperature factors were refined, with fixed unit-site occupancies, for the majority of H atoms. However, in the case of C(12) and C(13), the H atoms were refined with fixed isotropic thermal parameters.

A trial position for the Cl atom of 8OH-DPAT was found from a Patterson map using *SHELX*76 (Sheldrick, 1976), but a difference Fourier map calculated using this Cl was uninterpretable. A direct-methods approach using *SHELXS*86 (Sheldrick, 1986) located non-H atoms with the exception of the dipropylamino moiety. The structure was refined anisotropically by least squares (on F). Alternative positions for C(14)—C(15)—C(16) were tried by allowing half occupancies of both sites (these have been removed from Fig. 3 for the sake of clarity), but this model did not reduce the R factor beyond its final value of 0.1782. The data-collection output showed splitting of some peaks, consistent with a split (or possibly twinned) crystal, this resulted in the

Table 2. *Fractional coordinates and equivalent isotropic thermal parameters with e.s.d.'s for* 8MeO-PAT *and* 8OH-DPAT

$U_{eq} = (1/3)\sum_i\sum_j a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}/U_{iso}(Å^2)
8MeO-PAT				
Cl(1)	0.13545 (78)	0.14446 (8)	0.19762 (4)	0.0560 (5)
C(8)	0.5460 (3)	0.1811 (3)	−0.04343 (14)	0.0427 (14)
C(7)	0.6635 (3)	0.1004 (3)	−0.06686 (16)	0.0527 (17)
C(6)	0.7867 (3)	0.0886 (4)	−0.01817 (18)	0.0593 (18)
C(5)	0.7932 (3)	0.1558 (4)	0.05158 (18)	0.0588 (19)
C(10)	0.6736 (3)	0.2378 (3)	0.07585 (15)	0.0473 (15)
C(4)	0.6818 (3)	0.3099 (4)	0.15356 (17)	0.0600 (18)
C(3)	0.5317 (3)	0.3313 (3)	0.18427 (16)	0.0520 (16)
C(2)	0.4348 (3)	0.4157 (3)	0.12595 (14)	0.0405 (13)
C(1)	0.4126 (3)	0.3269 (3)	0.05184 (14)	0.0407 (14)
O(8)	0.41900 (19)	0.20087 (23)	−0.08653 (10)	0.0521 (11)
N(2)	0.29168 (22)	0.44585 (23)	0.15895 (11)	0.0420 (11)
C(9)	0.5493 (3)	0.2495 (3)	0.02850 (14)	0.0399 (13)
C(14)	0.4065 (4)	0.1313 (4)	−0.15965 (17)	0.0628 (19)
C(11)	0.1812 (3)	0.5283 (4)	0.10783 (17)	0.0585 (18)
C(12)	0.0527 (4)	0.5713 (5)	0.14748 (20)	0.0774 (23)
C(13)	−0.0613 (4)	0.6513 (6)	0.0976 (3)	0.097 (3)
H(71)	0.6594	0.0471	−0.1221	0.1140
H(61)	0.8792	0.0254	−0.0357	0.0677
H(51)	0.8907	0.1460	0.0884	0.0730
H(41)	0.7459	0.2378	0.1922	0.0671
H(42)	0.7336	0.4195	0.1502	0.0751
H(31)	0.5415	0.3961	0.2363	0.0795
H(32)	0.4847	0.2217	0.1952	0.0612
H(21)	0.4871	0.5212	0.1125	0.0611
H(11)	0.3758	0.4046	0.0074	0.0771
H(12)	0.3305	0.2414	0.0588	0.0668
H(22)	0.2455	0.3379	0.1737	0.0956
H(23)	0.3118	0.5131	0.2097	0.0613
H(141)	0.3005	0.1522	−0.1871	0.0860
H(142)	0.4255	0.0104	−0.1562	0.1211
H(143)	0.4885	0.1836	−0.1922	0.1007
H(111)	0.1473	0.4422	0.0699	0.0953
H(112)	0.2341	0.6197	0.0794	0.0967
8OH-DPAT				
Cl(1)	0.0662 (3)	0.19459 (24)	0.04771 (24)	0.0557 (19)
N(1)	0.2931 (15)	0.3392 (15)	0.1591 (14)	0.131 (14)
O(1)	0.4566 (16)	0.3621 (13)	−0.2217 (15)	0.172 (15)
C(1)	0.3558 (21)	0.3960 (18)	−0.0263 (22)	0.155 (21)
C(2)	0.3058 (21)	0.4272 (17)	0.0876 (18)	0.129 (18)
C(3)	0.1822 (22)	0.4847 (17)	0.0720 (21)	0.141 (20)
C(4)	0.2004 (20)	0.5766 (20)	0.0038 (19)	0.144 (20)
C(5)	0.2284 (14)	0.6174 (11)	−0.1947 (19)	0.142 (20)
C(6)	0.2803 (14)	0.5956 (11)	−0.2951 (19)	0.138 (20)
C(7)	0.3580 (14)	0.5111 (11)	−0.3054 (19)	0.143 (21)
C(8)	0.3838 (14)	0.4484 (11)	−0.2153 (19)	0.138 (21)
C(9)	0.3319 (14)	0.4703 (11)	−0.1148 (19)	0.119 (17)
C(10)	0.2542 (14)	0.5548 (11)	−0.1045 (19)	0.136 (21)
C(11)	0.207 (3)	0.341 (3)	0.2531 (24)	0.145 (5)
C(11′)	0.284 (5)	0.397 (4)	0.259 (5)	0.145 (5)
C(12)	0.249 (4)	0.426 (3)	0.334 (3)	0.145 (5)
C(12′)	0.150 (5)	0.350 (4)	0.323 (5)	0.145 (5)
C(13)	0.180 (4)	0.444 (3)	0.440 (3)	0.145 (5)
C(13′)	0.140 (5)	0.380 (4)	0.418 (5)	0.145 (5)
C(14)	0.424 (4)	0.280 (3)	0.156 (4)	0.145 (5)
C(14′)	0.913 (6)	0.219 (5)	−0.302 (5)	0.145 (5)
C(15)	0.417 (4)	0.191 (3)	0.246 (4)	0.145 (5)
C(15′)	0.929 (5)	0.324 (5)	−0.316 (5)	0.145 (5)
C(16)	0.548 (3)	0.138 (3)	0.234 (3)	0.145 (5)
C(16′)	0.918 (5)	0.434 (4)	−0.305 (4)	0.145 (5)

Table 3. *Selected angles and torsion angles* (°) *for* 8MeO-PAT *and* 8OH-DPAT

8MeO-PAT			
C(7)—C(8)—O(8)	124.06 (23)	C(8)—O(8)—C(14)	117.85 (21)
O(8)—C(8)—C(9)	114.74 (21)	C(2)—N(2)—C(11)	115.62 (20)
C(4)—C(3)—C(2)	109.19 (24)	C(8)—C(9)—C(1)	117.87 (22)
C(3)—C(2)—C(1)	111.95 (21)	C(10)—C(9)—C(1)	122.95 (23)
C(3)—C(2)—N(2)	108.63 (20)	N(2)—C(11)—C(12)	112.1 (3)
C(1)—C(2)—N(2)	110.38 (20)	C(11)—C(12)—C(13)	113.5 (3)
C(2)—C(1)—C(9)	113.17 (21)		
C(7)—C(8)—O(8)—C(14)	1.2 (4)	C(10)—C(3)—C(3)—C(2)	−52.7 (3)
C(9)—C(8)—O(8)—C(14)	−178.48 (23)	C(4)—C(3)—C(2)—C(1)	61.9 (3)
C(7)—C(8)—C(9)—C(1)	−175.98 (24)	C(4)—C(3)—C(2)—N(2)	−175.94 (21)
O(8)—C(8)—C(9)—C(10)	−179.07 (22)	C(3)—C(2)—C(1)—C(9)	−40.4 (3)
O(8)—C(8)—C(9)—C(1)	3.7 (3)	N(2)—C(2)—C(1)—C(9)	−161.54 (20)
C(6)—C(5)—C(10)—C(4)	179.3 (3)	C(3)—C(2)—N(2)—C(11)	−179.51 (22)
C(5)—C(10)—C(4)—C(3)	−154.8 (3)	C(1)—C(2)—N(2)—C(11)	−56.4 (3)
C(9)—C(10)—C(4)—C(3)	24.3 (4)	C(2)—C(1)—C(9)—C(8)	−171.99 (22)
C(5)—C(10)—C(9)—C(1)	175.07 (25)	C(2)—C(1)—C(9)—C(10)	10.9 (3)
C(4)—C(10)—C(9)—C(8)	179.87 (25)	C(2)—N(2)—C(11)—C(12)	−172.31 (24)
C(4)—C(10)—C(9)—C(1)	−3.0 (4)	N(2)—C(11)—C(12)—C(13)	−178.9 (3)
8OH-DPAT			
C(2)—N(1)—C(11)	121.4 (19)	O(1)—C(8)—C(7)	122.5 (17)
C(2)—N(1)—C(11′)	93.7 (26)	O(1)—C(8)—C(9)	117.5 (16)
C(2)—N(1)—C(14)	107.0 (21)	C(1)—C(9)—C(8)	116.3 (17)
C(11)—N(1)—C(14)	124.9 (24)	C(1)—C(9)—C(10)	123.6 (17)
C(11′)—N(1)—C(14)	114.7 (29)	C(4)—C(10)—C(5)	121.1 (17)
C(2)—C(1)—C(9)	114.5 (19)	C(4)—C(10)—C(9)	118.9 (17)
N(1)—C(2)—C(1)	110.3 (18)	N(1)—C(11)—C(12)	110.6 (25)
N(1)—C(2)—C(3)	113.3 (18)	C(11)—C(12)—C(13)	122.0 (29)
C(1)—C(2)—C(3)	110.7 (19)	N(1)—C(14)—C(15)	106.6 (29)
C(2)—C(3)—C(4)	112.0 (20)	C(14)—C(15)—C(16)	102.1 (31)
C(3)—C(4)—C(10)	112.78 (19)	C(14′)—C(15′)—C(16′)	163.3 (55)
C(11)—N(1)—C(2)—C(1)	−159.2 (22)	N(1)—C(2)—C(3)—C(4)	177.0 (18)
C(11)—N(1)—C(2)—C(3)	−34.4 (29)	C(1)—C(2)—C(3)—C(4)	−58.4 (25)
C(11′)—N(1)—C(2)—C(1)	165.4 (27)	C(2)—C(3)—C(4)—C(10)	54.5 (26)
C(11′)—N(1)—C(2)—C(3)	−69.8 (29)	C(3)—C(4)—C(10)—C(5)	153.8 (19)
C(14)—N(1)—C(2)—C(1)	48.2 (26)	C(3)—C(4)—C(10)—C(9)	−26.4 (27)
C(14)—N(1)—C(2)—C(3)	173.0 (23)	C(6)—C(5)—C(10)—C(4)	179.8 (18)
C(2)—N(1)—C(11)—C(12)	−56.1 (32)	C(6)—C(7)—C(8)—O(1)	178.0 (17)
C(14)—N(1)—C(11)—C(12)	91.4 (34)	O(1)—C(8)—C(9)—C(1)	−2.4 (26)
C(2)—N(1)—C(14)—C(15)	173.0 (24)	O(1)—C(8)—C(9)—C(10)	−178.1 (17)
C(11)—N(1)—C(14)—C(15)	21.6 (41)	C(7)—C(8)—C(9)—C(1)	175.6 (18)
C(11′)—N(1)—C(14)—C(15)	70.6 (39)	C(1)—C(9)—C(10)—C(4)	4.9 (29)
C(9)—C(1)—C(2)—N(1)	161.9 (18)	C(1)—C(9)—C(10)—C(5)	−175.3 (18)
C(9)—C(1)—C(2)—C(3)	35.6 (26)	C(8)—C(9)—C(10)—C(4)	−179.8 (18)
C(2)—C(1)—C(9)—C(8)	175.5 (17)	N(1)—C(11)—C(12)—C(13)	−178.7 (27)
C(2)—C(1)—C(9)—C(10)	−9.1 (29)		

failure of the structure to refine satisfactorily and the high $(\Delta/\sigma)_{max}$ value (Table 1).

Experimental data for both compounds are summarized in Table 1. The program *CALC* (Gould & Taylor, 1983) was used to provide the molecular geometry data presented in Table 3. Diagrams were prepared using *PLUTO* (Motherwell, 1972) and an interactive version of *ORTEP* (Johnson, 1965; Mallinson & Muir, 1985). Atomic scattering factors were from *International Tables for X-ray Crystallography* (1974, Vol. IV). The final atomic parameters for 8MeO-PAT and 8OH-DPAT are given in Table 2.*

Discussion. Crystallization of a racemic mixture of 8OH-DPAT was hindered as it easily oxidized in solution. One crystal was obtained from one sample and further crystallization attempts were unsuccessful. A previous crystal structure of 8OH-DPAT.HBr (Karlsson, Petterson, Sundell, Arvidsson & Hacksell, 1988) is of one enantiomer, (+)-8OH-DPAT.HBr, and shows two forms, differing in the position of the propyl side chains, in one asymmetric unit. A structure with the hydroxyl group transferred to C(5),

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54590 (27 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

5OH-DPAT.HCl [(+)-2-dipropylamino-5-hydroxytetralin hydrochloride], is also found to exist in two forms within the asymmetric unit, again differing in the positions of the propyl side chains (Giesecke, 1980). When 5OH-DPAT was methylated on C(3), (−)-C(3)Me-5OH-DPAT.HBr, only one form of one enantiomer was present in the asymmetric unit (Johansson, Nilsson, Karlen, Hacksell, Svensson, Carlsson, Kenne & Sundell, 1987). We tried to model the mobility of the propyl side chains of 8OH-DPAT by assigning half occupancies to C(11)—C(16) in their alternative positions, but this did not improve the model.

The bond lengths for both 8MeO-PAT and 8OH-DPAT were as expected. Selected bond and torsion angles for both crystal structures are given in Table 3. A comparison of the crystal structure of 8MeO-PAT with that of 5OH-DPAT (Giesecke, 1980), was made. Superimposing the aromatic rings clearly shows the ring pucker of the non-aromatic moiety such that only four out of the six C atoms in the non-aromatic ring superimpose. C(3) of 8MeO-PAT and the equivalent C atom of 5OH-DPAT (Fig. 1) lie 0.9 and 0.7 Å respectively out of the plane of the aromatic rings (Fig. 2). In both cases the N atom lies in the plane of C(3) resulting in similar angles at C(2)—C(3)—C(4) and C(2)—N(1)—C(11) (Table 3). The propyl group of 8MeO-PAT sits in the same position as one of the two 5OH-DPAT propyl groups. However, the atoms do not superimpose.

When the aromatic rings of 8OH-DPAT and 5OH-DPAT are superimposed, the positions of the N atoms again differ, resulting in a displacement of the propyl side chains, and the angles C(11)—N(1)—C(14) differ by 12° (Table 3). This is probably as a result of the poor model for 8OH-DPAT.

As expected, superimposing 8MeO-PAT and 8OH-DPAT gives a similar arrangement to those of each individually superimposed on 5OH-DPAT. However, superimposing along the N(1)—C(11) bond shows a deviation of 20° for the position of C(12) when viewed from the C(11) atom.

The molecular packing of 8MeO-PAT is shown in Fig. 3. Adjacent molecules packed in the same plane are rotated through 180° and sit head-to-tail, *i.e.* the propyl arm of one molecule points towards the methoxy group on the next. As a result, the methyl group is directed away from the non-aromatic ring, given a torsion angle of 1.2° between C(7), C(8), O(8) and C(14). There is no apparent hydrogen bonding between the O and the nearest H, on C(13). π–π ring stacking is present with a 3.7 Å spacing between the planes. The benzyl rings are displaced from one plane to the next by about 1.5 Å and are inverted. The position of the Cl ion influences the molecular packing of 8MeO-PAT since salt bridges are formed between N—H and Cl, with an N to Cl distance of 3.12 Å. The H associated with Cl links with the adjacent molecule's H—N forming a chain through the crystal.

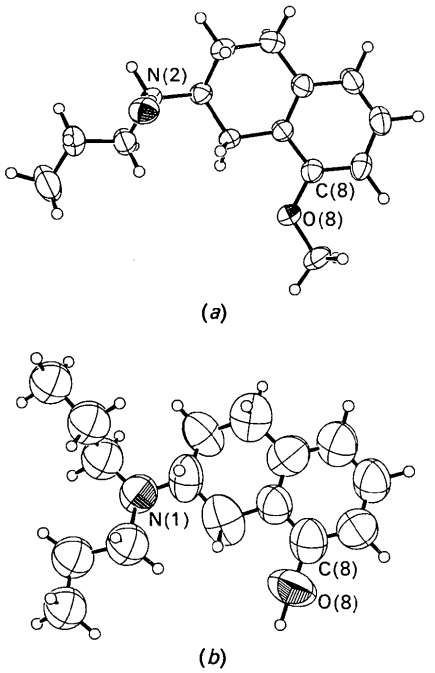

Fig. 2. Perspective drawing of (*a*) 8MeO-PAT and (*b*) 8OH-DPAT. Non-H atoms are shown as 50% probability thermal ellipsoids; Cl, O and N atoms are shaded.

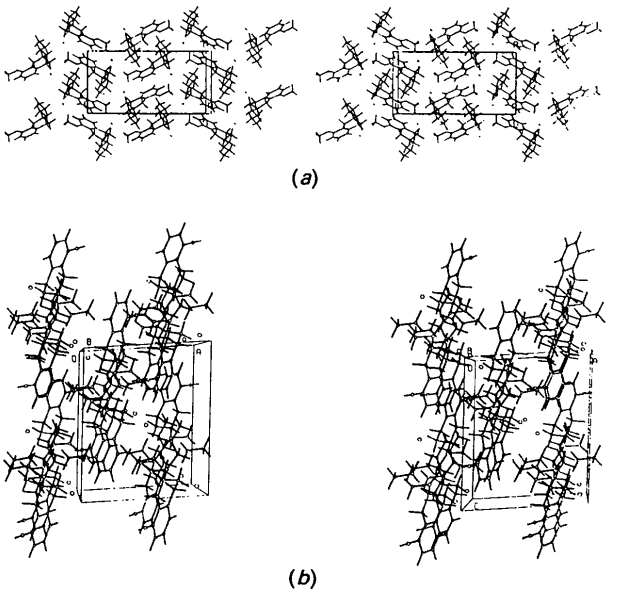

Fig. 3. Molecular packing of (*a*) 8MeO-PAT (projection is down the *c* axis) and (*b*) 8OH-DPAT (projection is down the *b* axis).

The molecular packing of 8OH-DPAT showed that there are few close contacts between molecules. The molecules lie in an infinite stack with pairs of molecules related by inversion centres. The propyl arms are badly disordered; this hindered the search for close contacts between the molecules. It is possible that there is a similar salt-bridge effect to that found in 8MeO-PAT although the distances are a little long. The C(11), C(12) and C(13) propyl chain is closer to the nearest Cl ion than the C(14)—C(16) propyl chain; the H atoms on C(11) come within 3 Å of the Cl ion. The other closest atoms to the Cl ion are the H atoms bound to C(6) and C(7).

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Mesoionic Compounds. 2. Structure of 2-Morpholino-5-propyl-1,3-dithiolium-4-thiolate

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Abstract. $C_{10}H_{15}NOS_3$, $M_r = 261.43$, monoclinic, $P2_1/c$, $a = 7.511$ (1), $b = 10.088$ (1), $c = 17.383$ (1) Å, $\beta = 112.41$ (1)°, $V = 1217.7$ (4) Å^3, $Z = 4$, $D_x = 1.426$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 5.6$ cm^{-1}, $F(000) = 552$, $T = 297$ K, $R = 0.030$ for 1339 reflections with $|F_o| > 3\sigma(|F_o|)$. In the pentatomic ring

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