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Structure and Conductivity of a New Phase of 3,4;3′,4′-Bis(ethylenedithio)-2,2′,5,5′-tetrathiafulvalene Hexafluorophosphate: γ-(BEDT-TTF)$_2$PF$_6$

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Abstract. γ-$(C_{10}H_8S_8)_2PF_6$, $M_r = 914.34$, triclinic, $P\bar{1}$, $a = 6.607$ (2), $b = 14.988$ (2), $c = 16.803$ (3) Å, $\alpha = 78.27$ (1), $\beta = 88.55$ (2), $\gamma = 87.78$ (2)°, $V = 1627.8$ (8) Å^3, $Z = 2$, $D_x = 1.87$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 11.22$ cm^{-1}, $F(000) = 922$, room temperature, $R(F) = 0.050$, $wR(F) = 0.063$ for 3768 unique reflections. The structure consists of layers of BEDT-TTF cations with a formal charge of +0.5. The slightly disordered PF_6^- anions are located in layers between the BEDT-TTF sheets. The packing is compared with that in the previously reported α and β phases. Conductivity measurements indicate γ-$(C_{10}H_8S_8)_2PF_6$ to be a semiconductor with a band gap of 60–80 meV.

Introduction. Salts of BEDT-TTF are of particular interest because of their unusual solid-state properties. The organic superconductors with highest T_c known to date, such as κ-(BEDT-TTF)$_2$[Cu(NCS)$_2$] (Saito, Urayama, Yamochi & Oshima, 1988), κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br and κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl (Wang *et al.*, 1991; Kini *et al.*, 1990) belong to this class.

The present paper is one in a continuing series describing products of electrocrystallization reactions, aimed at the synthesis of novel salts, and the study of the relationship between structure and properties. Previous papers in this series concern (BEDT-TTF)$_2$HgBr$_4$(TCE) (Bu, Coppens & Naughton, 1990), (BEDT-TTF)$_2$Cd$_2$I$_6$ (Bu, Su & Coppens, 1991) and β-(BEDT-TTF)$_2$CuCl$_2$ (Bu, Coppens, Lederle & Naughton, 1991).

Experimental. Crystals of γ-(BEDT-TTF)$_2$PF$_6$ have been prepared in an attempt to synthesize (BEDT-TTF)$_2$CuSCNBr, which was expected to have a structure similar to the κ-phase superconductor (BEDT-TTF)$_2$Cu(SCN)$_2$. Electrocrystallization was performed in a mixed solvent of 1,1,2-trichloroethane (TCE) and 10% volume absolute ethanol, containing 1 m*M* BEDT-TTF, 2 m*M* CuSCN, 2 m*M* KBr, 10 m*M* 18-crown-6 and 0.1 *M* [CH$_3$(CH$_2$)$_3$]$_4$NPF$_6$ as supporting electrolyte. A current of 6.0 μA was applied to a 40 ml solution. Crystals were collected after 2 days. Although we had successfully employed the supporting electrolyte [CH$_3$(CH$_2$)$_3$]$_4$NPF$_6$ in the earlier preparations of (BEDT-TTF)$_2$HgBr$_4$(TCE) (Bu, Coppens & Naughton, 1990), and other novel solids, a previously unknown phase of (BEDT-TTF)$_2$PF$_6$ was obtained in the present experiment.

A single crystal of γ-(BEDT-TTF)$_2$PF$_6$, with dimensions 0.48 × 0.13 × 0.075 mm, was mounted on a glass fiber. Unit-cell dimensions were determined by least-squares refinement of the setting angles of 25 reflections ($20 < 2\theta < 32°$). Room-temperature data were collected on a MicroVAX-controlled CAD-4 diffractometer with the $\theta/2\theta$ scan technique and graphite-monochromatized Mo $K\alpha$ radiation (λ = 0.71073 Å). Three standard reflections monitored throughout the data collection showed less than 2% change in intensity. 6368 reflections with $2 < \theta < 25°$ were measured ($h = 0, 7$; $k = -17, 17$; $l = -19, 19$) and averaged to give 5698 unique reflections, the internal agreement factor $R(F) = 0.016$. Data were reduced using the VAX *SDP* (Enraf–Nonius, 1985) package. Numerical absorption corrections were applied (Coppens, Leiserowitz & Rabinovich, 1965). The transmission factors ranged from 0.80 to 0.93. The structure was solved based on the non-centrosymmetric space group *P*1 using *MULTAN*11/82 in the *SDP* package. Upon examination of the refined atomic parameters in the *P*1 space group the centrosymmetric nature of the structure was evident. The presence of a center of symmetry was supported by the intensity statistics. 3768 unique reflections with $I > 3\sigma(I)$ were used in the final full-matrix refinement with anisotropic thermal parameters for all non-H atoms. The positions of H atoms were calculated using a C—H distance of 0.95 Å and

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included in the structure-factor calculation. A total of 388 variables were refined, minimizing the function $\sum[w(|F_{\rm obs}| - k|F_{\rm cal}|)^2]$, where $w = 1/\sigma^2(F)$; $\sigma(F) = \sigma(F^2)/2F$; $\sigma(F^2) = [\sigma^2_{\rm counting} + (0.02|F|^2)^2]^{1/2}$. Scattering factors (including anomalous contributions) were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Parameter shifts in the final least-squares cycle were smaller than 0.02σ. For 3768 reflections, $R(F) = 0.050$, $wR(F) = 0.063$, GOF = 3.07.

Final atomic coordinates and equivalent isotropic thermal parameters are listed in Table 1,* while bond lengths and angles are given in Tables 2 and 3 respectively. Fig. 1 shows the atomic labelling scheme for the BEDT-TTF molecule and Fig. 2 is the packing diagram projected down the *a* axis.

Discussion. The unit cell contains four BEDT-TTF molecules and two PF_6^- anions. BEDT-TTF molecules are stacked along the *b* axis. The intrastack packing mode is type *c* according to the classification of Williams *et al.* (1987), with a rotation of the two molecules relative to each other. The in-plane molecular axes of the two adjacent BEDT-TTF molecules make an angle as large as 23° (calculated from two central C=C bonds). The stacks are interlinked by short S···S contacts. The shortest interstack S···S distance is 3.430 (2) Å, which is less than the van der Waals radii sum of 3.6 Å. The interstack packing mode is of type *l* in terms of the same classification. The six F atoms in PF_6^- anions have large thermal parameters indicating these anions undergo very large thermal oscillations. The anisotropic thermal parameters for C atoms in ethylene groups correspond to large displacements in a direction perpendicular to the BEDT-TTF molecular plane, likely corresponding to static disorder, as often observed in BEDT-TTF salts (Williams *et al.*, 1987).

Two phases of $(BEDT\text{-}TTF)_2PF_6$ have been reported previously (Kobayashi, Kato *et al.*, 1983; Kobayashi, Mori *et al.*, 1983). In α-$(BEDT\text{-}TTF)_2PF_6$, the intrastack packing is of the *a* mode corresponding to a relative shift along the long molecular axis, while in β-$(BEDT\text{-}TTF)_2PF_6$, the *c* and *l* modes are adopted for intra- and interstack packing respectively. In the orthorhombic β phase the molecular planes of the BEDT-TTF molecules in adjacent layers form a herringbone pattern, unlike the parallel arrangements found in the α and γ phases. The volume of a structural unit consisting of two BEDT-TTF molecules and one PF_6 anion is the

* Lists of structure factors and thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54556 (23 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CR0328]

Table 1. *Positional parameters and equivalent isotropic thermal parameters* (Å^2) *with e.s.d.'s in parentheses*

	x	*y*	*z*	B_{eq}*
P1	0.3295 (3)	0.2420 (2)	0.4938 (1)	4.37 (4)
S1	−0.2134 (2)	0.1400 (1)	−0.01582 (8)	3.40 (3)
S2	0.2125 (2)	0.1290 (1)	−0.06652 (8)	3.52 (3)
S3	−0.0906 (2)	0.0562 (1)	0.16902 (8)	3.11 (3)
S4	0.3366 (2)	0.0532 (1)	0.12017 (9)	3.87 (3)
S5	−0.3617 (2)	0.2298 (1)	−0.17576 (9)	4.35 (4)
S6	0.1461 (2)	0.2124 (1)	−0.23840 (9)	4.14 (4)
S7	−0.0191 (2)	0.0002 (2)	0.34410 (9)	5.34 (5)
S8	0.4882 (2)	−0.0099 (1)	0.28618 (9)	4.32 (4)
C1	0.0366 (7)	0.1106 (4)	0.0124 (3)	2.8 (1)
C2	0.0871 (8)	0.0783 (3)	0.0909 (3)	2.7 (1)
C3	−0.1519 (8)	0.1858 (4)	−0.1173 (3)	2.9 (1)
C4	0.0408 (8)	0.1812 (4)	−0.1409 (3)	2.9 (1)
C5	0.0849 (8)	0.0250 (4)	0.2469 (3)	2.9 (1)
C6	0.2819 (7)	0.0224 (4)	0.2233 (3)	3.0 (1)
C7	−0.259 (1)	0.2358 (7)	−0.2755 (4)	7.9 (3)
C8	−0.067 (1)	0.2495 (8)	−0.2955 (5)	9.5 (3)
C9	0.197 (1)	−0.0300 (6)	0.4081 (4)	5.7 (2)
C10	0.386 (1)	0.0157 (5)	0.3782 (4)	5.2 (2)
S1*b*	−0.1373 (2)	0.4700 (1)	−0.17516 (8)	3.44 (3)
S2*b*	0.2806 (2)	0.4143 (1)	−0.13122 (9)	3.67 (3)
S3*b*	−0.2785 (2)	0.3948 (1)	0.01234 (9)	3.67 (3)
S4*b*	0.1442 (2)	0.3451 (1)	0.05348 (9)	3.64 (3)
S5*b*	−0.0525 (2)	0.5288 (1)	−0.34996 (9)	4.35 (4)
S6*b*	0.4456 (3)	0.4617 (2)	−0.2974 (1)	6.76 (6)
S7*b*	−0.4410 (3)	0.3291 (2)	0.1767 (1)	6.52 (5)
S8*b*	0.0650 (2)	0.2698 (1)	0.22642 (9)	3.82 (3)
C1*b*	0.0298 (8)	0.4222 (4)	−0.0997 (3)	2.7 (1)
C2*b*	−0.0291 (8)	0.3912 (4)	−0.0207 (3)	2.9 (1)
C3*b*	0.0433 (8)	0.4837 (4)	−0.2539 (3)	3.0 (1)
C4*b*	0.2348 (9)	0.4571 (4)	−0.2336 (3)	3.6 (1)
C5*b*	−0.2298 (8)	0.3419 (4)	0.1126 (3)	3.5 (1)
C6*b*	−0.0327 (8)	0.3189 (4)	0.1320 (3)	3.0 (1)
C7*b*	0.166 (1)	0.5364 (7)	−0.4141 (4)	7.4 (2)
C8*b*	0.339 (1)	0.4815 (8)	−0.3921 (5)	8.8 (3)
C9*b*	−0.349 (1)	0.2510 (6)	0.2594 (5)	7.0 (2)
C10*b*	−0.156 (1)	0.2642 (6)	0.2920 (4)	5.9 (2)
F1	0.1309 (8)	0.2916 (5)	0.5085 (3)	13.1 (2)
F2	0.416 (1)	0.3351 (4)	0.4675 (5)	16.3 (3)
F3	0.5315 (8)	0.1947 (5)	0.4759 (4)	12.0 (2)
F4	0.244 (1)	0.1471 (4)	0.5167 (4)	15.0 (2)
F5	0.2705 (8)	0.2472 (4)	0.4027 (3)	9.1 (1)
F6	0.374 (1)	0.2322 (4)	0.5850 (3)	12.0 (2)

* Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: $B_{eq} = \frac{1}{3}\sum_i\sum_j B_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

Table 2. *Bond distances* (Å)

P1—F1	1.523 (6)	C5—C6	1.353 (7)
P1—F2	1.504 (7)	C7—C8	1.31 (1)
P1—F3	1.539 (6)	C9—C10	1.476 (9)
P1—F4	1.523 (7)	S1*b*—C1*b*	1.726 (5)
P1—F5	1.574 (5)	S1*b*—C3*b*	1.745 (5)
P1—F6	1.545 (5)	S2*b*—C1*b*	1.734 (5)
S1—C1	1.745 (5)	S2*b*—C4*b*	1.740 (5)
S1—C3	1.748 (5)	S3*b*—C2*b*	1.727 (5)
S2—C1	1.727 (5)	S3*b*—C5*b*	1.742 (5)
S2—C4	1.751 (5)	S4*b*—C2*b*	1.735 (5)
S3—C2	1.728 (5)	S4*b*—C6*b*	1.734 (5)
S3—C5	1.751 (5)	S5*b*—C3*b*	1.742 (5)
S4—C2	1.738 (5)	S5*b*—C7*b*	1.774 (7)
S4—C6	1.732 (5)	S6*b*—C4*b*	1.730 (6)
S5—C3	1.748 (5)	S6*b*—C8*b*	1.723 (8)
S5—C7	1.778 (7)	S7*b*—C5*b*	1.733 (6)
S6—C4	1.745 (5)	S7*b*—C9*b*	1.732 (8)
S6—C8	1.735 (8)	S8*b*—C6*b*	1.737 (5)
S7—C5	1.730 (5)	S8*b*—C10*b*	1.799 (7)
S7—C9	1.795 (7)	C1*b*—C2*b*	1.366 (7)
S8—C6	1.739 (5)	C3*b*—C4*b*	1.343 (8)
S8—C10	1.779 (7)	C5*b*—C6*b*	1.364 (7)
C1—C2	1.355 (7)	C7*b*—C8*b*	1.39 (1)
C3—C4	1.327 (7)	C9*b*—C10*b*	1.44 (1)

Intermolecular S···S distances less than 3.6 Å

S2—S5^{i}	3.537 (2)	S1*b*—S6*b*^{ii}	3.500 (2)
S3—S8^{ii}	3.428 (2)	S4*b*—S7*b*^{i}	3.448 (2)
S5—S6^{ii}	3.479 (2)	S5*b*—S6*b*^{ii}	3.541 (2)
S7—S8^{ii}	3.439 (2)	S7*b*—S8*b*	3.454 (2)

Symmetry codes: (i) $x + 1, y, z$; (ii) $x - 1, y, z$.

Table 3. *Bond angles* (°)

F1—P1—F2	86.3 (4)	F1—P1—F3	177.8 (3)
F1—P1—F4	94.8 (4)	F1—P1—F5	90.1 (3)
F1—P1—F6	88.1 (3)	F2—P1—F3	92.0 (4)
F2—P1—F4	177.5 (5)	F2—P1—F5	88.0 (4)
F2—P1—F6	95.8 (4)	F3—P1—F4	86.8 (4)
F3—P1—F5	88.4 (3)	F3—P1—F6	93.5 (3)
F4—P1—F5	89.8 (4)	F4—P1—F6	86.5 (5)
F5—P1—F6	175.7 (3)	C1—S1—C3	94.7 (2)
C1—S2—C4	95.7 (2)	C2—S3—C5	95.8 (2)
C2—S4—C6	95.6 (2)	C3—S5—C7	100.6 (3)
C4—S6—C8	101.5 (3)	C5—S7—C9	103.8 (3)
C6—S8—C10	99.8 (3)	S1—C1—S2	115.0 (3)
S1—C1—C2	121.8 (4)	S2—C1—C2	123.2 (4)
S3—C2—S4	114.9 (3)	S3—C2—C1	122.9 (4)
S4—C2—C1	122.2 (4)	S1—C3—S5	113.6 (3)
S1—C3—C4	117.9 (4)	S5—C3—C4	128.5 (4)
S2—C4—S6	114.6 (3)	S2—C4—C3	116.5 (4)
S6—C4—C3	128.7 (4)	S3—C5—S7	115.0 (3)
S3—C5—C6	116.0 (4)	S7—C5—C6	128.9 (4)
S4—C6—S8	116.1 (3)	S4—C6—C5	117.5 (4)
S8—C6—C5	126.4 (4)	S5—C7—C8	124.3 (6)
S6—C8—C7	128.8 (6)	S7—C9—C10	116.0 (4)
S8—C10—C9	115.3 (6)	C1*b*—S1*b*—C3*b*	95.4 (2)
C1*b*—S2*b*—C4*b*	95.3 (3)	C2*b*—S3*b*—C5*b*	95.4 (2)
C2*b*—S4*b*—C6*b*	95.9 (2)	C3*b*—S5*b*—C7*b*	103.3 (3)
C4*b*—S6*b*—C8*b*	102.2 (3)	C5*b*—S7*b*—C9*b*	101.3 (3)
C6*b*—S8*b*—C10*b*	102.5 (3)	S1*b*—C1*b*—S2*b*	115.3 (3)
S1*b*—C1*b*—C2*b*	123.1 (4)	S2*b*—C1*b*—C2*b*	121.7 (4)
S3*b*—C2*b*—S4*b*	115.4 (3)	S3*b*—C2*b*—C1*b*	123.0 (4)
S4*b*—C2*b*—C1*b*	121.6 (4)	S1*b*—C3*b*—S5*b*	114.7 (3)
S1*b*—C3*b*—C4*b*	116.8 (4)	S5*b*—C3*b*—C4*b*	128.5 (4)
S2*b*—C4*b*—S6*b*	115.3 (3)	S2*b*—C4*b*—C3*b*	117.1 (4)
S6*b*—C4*b*—C3*b*	127.7 (4)	S3*b*—C5*b*—S7*b*	114.8 (3)
S3*b*—C5*b*—C6*b*	117.1 (4)	S7*b*—C5*b*—C6*b*	128.0 (4)
S4*b*—C6*b*—S8*b*	115.6 (3)	S4*b*—C6*b*—C5*b*	116.3 (4)
S8*b*—C6*b*—C5*b*	128.1 (4)	S5*b*—C7*b*—C8*b*	121.4 (6)
S6*b*—C8*b*—C7*b*	124.7 (7)	S7*b*—C9*b*—C10*b*	119.6 (6)
S8*b*—C10*b*—C9*b*	118.7 (5)		

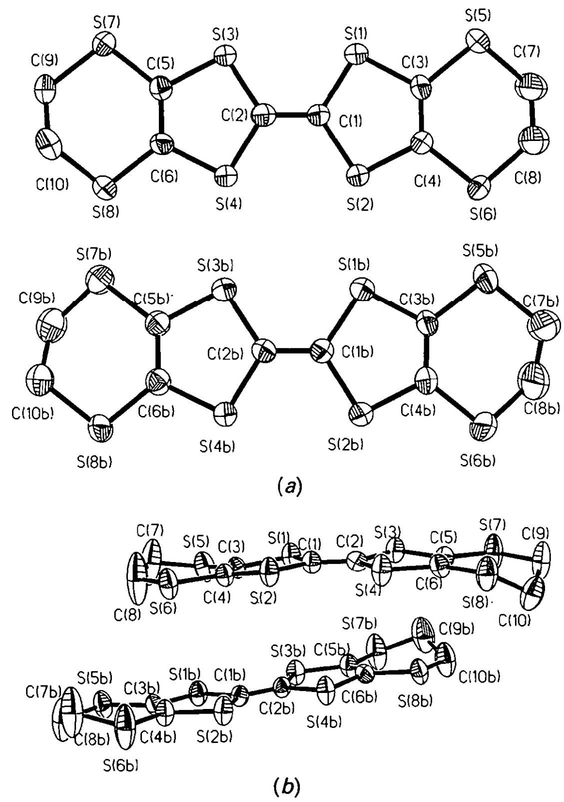

Fig. 1. (*a*) Top and (*b*) side views, with atomic labelling, of the two crystallographically independent BEDT-TTF molecules. Thermal ellipsoids are drawn at the 50% level.

same in the β and γ phases (814 Å^3), but somewhat lower (794 Å^3) for the more efficient packing of the α phase. In all cases the PF_6^- ions are located in a plane between the BEDT-TTF sheets. The versatility of the BEDT-TTF molecule in forming salts with different packing modes is one of the reasons behind the remarkable variety of electrical properties in the BEDT-TTF family (Williams *et al.*, 1987).

Four-probe measurements of the conductivity along the needle (*a*) axis were performed on a single crystal. The resistivity of γ-(BEDT-TTF)$_2$PF$_6$ in the temperature range 140 to 290 K is shown in Fig. 3. It is found that log ρ is linear in T in most of the temperature range studied (open circles). Though the $1/T$ range over which measurements were made is rather small, because of the rapidly increasing resistance, the data can also be interpreted as representing traditional semiconducting behaviour, $\rho \sim e^{\Delta/T}$, but with a temperature-dependent gap $\Delta(T)$ which varies between 60 and 80 meV.

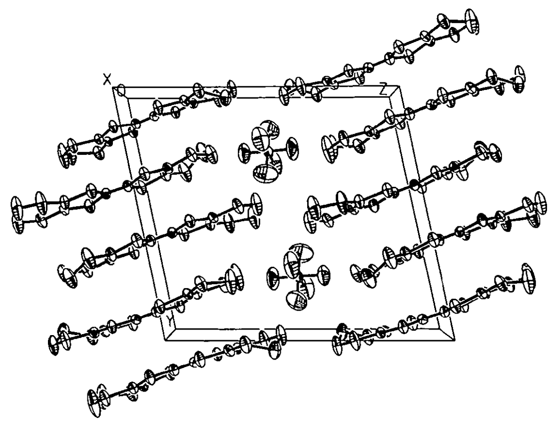

Fig. 2. Crystal structure projected onto the *bc* plane. Thermal ellipsoids are drawn at the 50% level.

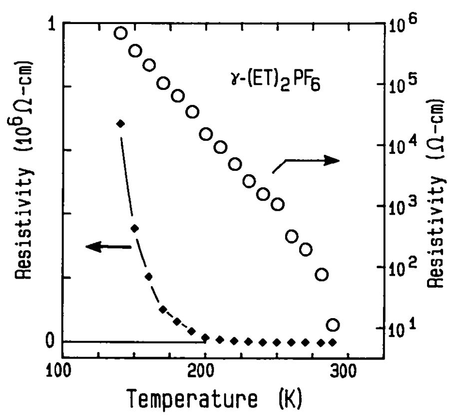

Fig 3 Resistivity as a function of T on a linear scale (left) and a logarithmic scale (right).

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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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