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# 3,4-Pyrazino-3′,4′-ethylenedithio-2,2′,5,5′-tetrathiafulvalenium[†] Tetraiodothallate(III) Solvate (3:1) with 1,1,2-Trichloroethane, (PEDT–TTF)$_3$TlI$_4$.TCE

Urs Geiser, John A. Schlueter, Aravinda M. Kini, Crystal A. Achenbach, Adam S. Komosa and Jack M. Williams

*Chemistry & Materials Science Divisions, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439, USA*

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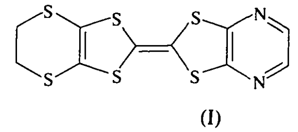
## Abstract

The organic donor molecule PEDT–TTF (3,4-pyrazino-3′,4′-ethylenedithio-2,2′,5,5′-tetrathiafulvalene) forms a semiconducting 3:1 solvate salt with $\mathrm{TlI_4^-}$ in TCE (1,1,2-trichloroethane), $(\mathrm{C_{10}H_6N_2S_6})_3^+.\mathrm{TlI_4^-}.\mathrm{C_2H_3Cl_3}$. Its crystal structure contains stacks with six sinusoidally displaced PEDT–TTF molecules per repeat unit. However, the topology of short intermolecular S···S interactions is one dimensional in the transverse direction which coincides with the direction of the most developed crystal growth.

## Comment

Over 50 organic superconductors are based on the electron-donor molecule bis(ethylenedithio)tetrathiafulvalene, or ET (for a review, see Williams *et al.*, 1992). Salts of many related donor molecules have been synthesized, but these have yielded much fewer superconductors to date. One of these modified donor molecules is PEDT–TTF, 3,4-pyrazino-3′,4′-ethylenedithio-2,2′,5,5′-tetrathiafulvalene, which we chose to study because of its oxidation potential that is similar to that of ET. Previously reported salts of this donor are: (PEDT–TTF)$_2$PF$_6$ and (PEDT–TTF)$_2$BF$_4$(CH$_2$Cl$_2$)$_{0.5}$ (Mentzafos, Psycharis & Terzis, 1989), (PEDT–TTF)$_2$IBr$_2$ (Terzis, Psycharis, Hountas & Papavassiliou, 1988) and (PEDT–TTF)$_2$(I$_3$)$_{2/3}$ (Psycharis, Hountas, Terzis & Papavassiliou, 1988). Electrocrystallization with tetra(*n*-butyl)ammonium tetraiodothallate(III) in TCE (TCE = 1,1,2-trichloroethane) on platinum electrodes yielded black elongated hexagonal plates of the title compound, (I). One of these plates was cut to a size suitable for an X-ray structure determination.



$.\mathrm{TlI_4.C_2H_3Cl_3}$

(I)

The crystal structure contains three crystallographically independent PEDT–TTF molecules (Fig. 1), a tetrahedral $\mathrm{TlI_4^-}$ anion and a disordered solvent molecule, all in general positions. As seen in Fig. 2, the electron-donor molecules stack along the *c* direction with six molecules per repeat unit in the pattern *ABCC′B′A′* (*A*, *B* and *C* denote the independent PEDT–TTF moieties 2, 3 and 1, respectively, and primes indicate inversion symmetric equivalents). All donor molecules are essentially coplanar, with the plane normal inclined with respect to the stacking direction by *ca* 17–20°. While the dimers *A′A* and *CC′* are located directly on the stacking axis, the molecules *B* and *B′* are offset by ±3.8 Å along **b** from the stacking axis, thus a transverse sinusoidal displacement is discernible in the stack (see Fig. 2). The orientation of the ethylenedithio and pyrazino end groups alternates along the stacking direction.

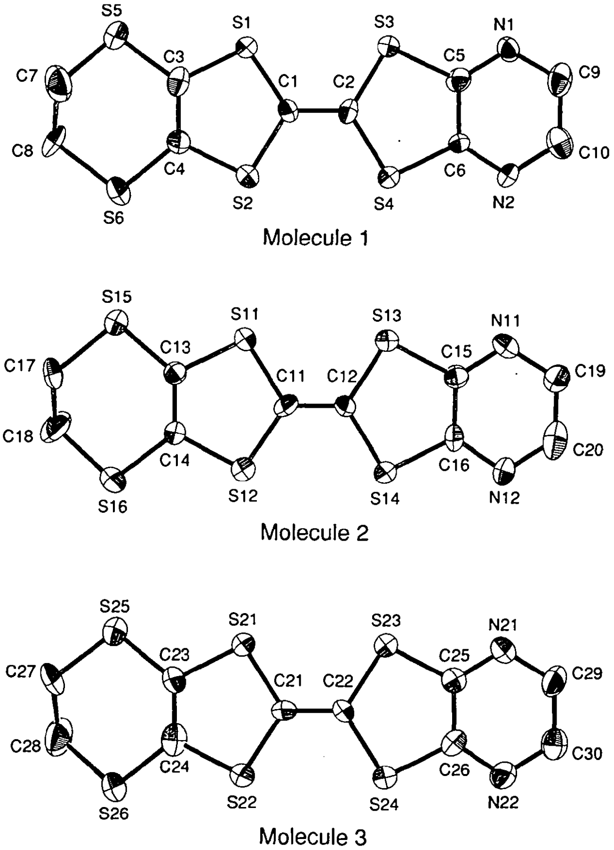


Fig. 1. The three crystallographically independent PEDT–TTF molecules in (PEDT–TTF)$_3$TlI$_4$.TCE with atomic labels. Displacement ellipsoids are drawn at the 50% probability level.

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[†] IUPAC recommended name: (2-dithiolo[4,5-*b*]dithiin-2-ylidene)dithiolo[4,5-*b*]pyrazinium.

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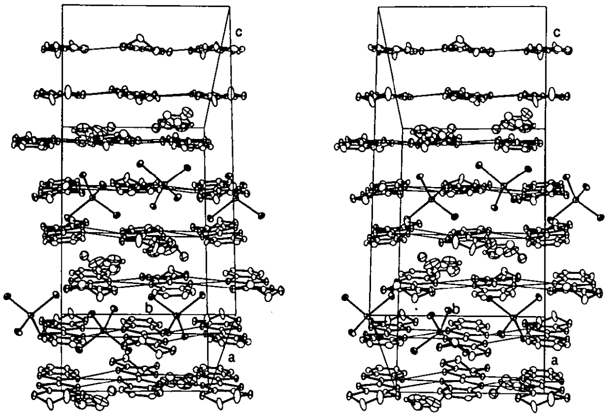

Fig. 2. Stereoview of the unit cell of (PEDT–TTF)$_3$TlI$_4$.TCE projected approximately along the long molecular axes of the PEDT–TTF moieties. The anion/solvent layer at $x \simeq 0.0$ is omitted for clarity. Intermolecular S···S contacts shorter than 3.6 Å are drawn as thin lines and the atoms are shown as 20% probability ellipsoids.

The chemically equivalent bonds of all three PEDT–TTF molecules are of equal length within experimental uncertainty. The lengths of the central C=C bond and the inner C—S bonds of similar molecules are indicative of the charge of the molecule (Williams *et al.*, 1992). The bond lengths in the title compound are intermediate between those found in neutral ET and ET$^{+1/2}$, thus the average +1/3 charge is equally distributed over the three crystallographically independent molecules.

Two PEDT–TTF molecular stacks, related by the screw rotation, are found in the unit cell. The short intermolecular interactions, with distances less than the sum of the van der Waals radii (Bondi, 1964), occur in ribbons along **b** and are thus perpendicular to the stacking direction *c*, see Fig. 2. This topology of short contacts suggests that the crystals are most conducting along the *b* direction. The resistivity measured (four probe, DC method) along that direction was semiconducting within the temperature range 15–300 K with $\rho_{300} = 0.25\ \Omega$ m. The stacks together form a donor-molecule layer in the *bc* plane centered at $x = 0.5$. These layers are separated by a mixed anion–solvent layer at $x = 0$. The anion is a regular tetrahedron with average Tl—I bond lengths of 2.763 (3) Å, in good agreement with other structures containing the same anion (Thiele, Rotter & Zimmermann, 1986; Beno *et al.*, 1987). A disordered model with two conformations was refined for the TCE solvent molecule.

## Experimental

### *Crystal data*

$3C_{10}H_6N_2S_6.TlI_4.C_2H_3Cl_3$
$M_r = 1884.95$
Monoclinic
$P2_1/c$
$a = 20.155\ (6)$ Å
$b = 12.151\ (2)$ Å
$c = 22.026\ (4)$ Å
$\beta = 99.81\ (2)°$
$V = 5315\ (2)$ Å$^3$
$Z = 4$
$D_x = 2.356$ Mg m$^{-3}$

Mo $K\alpha$ radiation
$\lambda = 0.7107$ Å
Cell parameters from 22 reflections
$\theta = 10.8–15.3°$
$\mu = 6.24$ mm$^{-1}$
$T = 298$ K
Cut plate
0.28 × 0.23 × 0.07 mm
Black
Crystal source: synthesized by electrocrystallization

### *Data collection*

Syntex $P2_1$ diffractometer
$\omega$ scans
Absorption correction: by integration from crystal shape
$T_{\min} = 0.261$, $T_{\max} = 0.667$
11311 measured reflections
9354 independent reflections
5970 observed reflections [$I > 2\sigma(I)$]

$R_{\text{int}} = 0.027$
$\theta_{\max} = 25°$
$h = -1 \rightarrow 23$
$k = -14 \rightarrow 0$
$l = -26 \rightarrow 25$
3 standard reflections monitored every 58 reflections intensity decay: 5% corrected

### *Refinement*

Refinement on $F$
$R = 0.070$
$wR = 0.051$
$S = 1.77$
5970 reflections
585 parameters
H atoms not included
$w = 1/\sigma^2(F)$

$(\Delta/\sigma)_{\max} = 0.25$
$\Delta\rho_{\max} = 1.5$ e Å$^{-3}$
$\Delta\rho_{\min} = -1.2$ e Å$^{-3}$
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å$^2$)*

$$U_{\text{eq}} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

| | $x$ | $y$ | $z$ | $U_{\text{eq}}$ |
|---|---|---|---|---|
| Tl | 0.00264 (3) | 0.21247 (6) | 0.27810 (3) | 0.0503 (2) |
| I1 | −0.09975 (6) | 0.29064 (11) | 0.18920 (5) | 0.0743 (5) |
| I2 | 0.04524 (7) | 0.38038 (11) | 0.36009 (5) | 0.0784 (5) |
| I3 | 0.11394 (6) | 0.14430 (10) | 0.23033 (5) | 0.0648 (5) |
| I4 | −0.04641 (6) | 0.04034 (10) | 0.33983 (5) | 0.0698 (5) |
| S1 | 0.6418 (2) | 0.1042 (3) | 0.4740 (2) | 0.0386 (14) |
| S2 | 0.6351 (2) | −0.1352 (3) | 0.4870 (2) | 0.0379 (13) |
| S3 | 0.4869 (2) | 0.1075 (3) | 0.4049 (2) | 0.0380 (13) |
| S4 | 0.4821 (2) | −0.1361 (3) | 0.4174 (2) | 0.0377 (13) |
| S5 | 0.7826 (2) | 0.1248 (3) | 0.5386 (2) | 0.051 (2) |
| S6 | 0.7738 (2) | −0.1635 (3) | 0.5515 (2) | 0.054 (2) |
| N1 | 0.3589 (6) | 0.1009 (9) | 0.3442 (5) | 0.036 (4) |
| N2 | 0.3561 (6) | −0.1329 (9) | 0.3544 (5) | 0.035 (4) |
| C1 | 0.5939 (6) | −0.0137 (10) | 0.4607 (5) | 0.030 (5) |
| C2 | 0.5283 (6) | −0.0144 (11) | 0.4310 (6) | 0.032 (5) |
| C3 | 0.7139 (7) | 0.0392 (12) | 0.5122 (6) | 0.038 (5) |
| C4 | 0.7111 (7) | −0.0727 (11) | 0.5177 (6) | 0.036 (5) |
| C5 | 0.4115 (7) | 0.0431 (11) | 0.3721 (6) | 0.034 (5) |
| C6 | 0.4092 (7) | −0.0744 (10) | 0.3770 (6) | 0.030 (5) |
| C7 | 0.8515 (8) | 0.0260 (14) | 0.5401 (7) | 0.060 (7) |
| C8 | 0.8447 (7) | −0.0723 (13) | 0.5816 (7) | 0.059 (7) |
| C9 | 0.3031 (8) | 0.0435 (14) | 0.3201 (6) | 0.046 (6) |
| C10 | 0.3018 (8) | −0.0737 (13) | 0.3251 (6) | 0.044 (6) |
| S11 | 0.5879 (2) | 0.1046 (3) | 0.1246 (2) | 0.0384 (13) |
| S12 | 0.5901 (2) | −0.1355 (3) | 0.1192 (2) | 0.0399 (14) |
| S13 | 0.4333 (2) | 0.1061 (3) | 0.0576 (2) | 0.0404 (14) |
| S14 | 0.4367 (2) | −0.1372 (3) | 0.0487 (2) | 0.0395 (13) |

| | | | | |
|---|---|---|---|---|
| S15 | 0.7289 (2) | 0.1315 (3) | 0.1817 (2) | 0.051 (2) |
| S16 | 0.7301 (2) | −0.1596 (3) | 0.1837 (2) | 0.054 (2) |
| N11 | 0.3029 (6) | 0.0998 (9) | 0.0041 (5) | 0.038 (4) |
| N12 | 0.3058 (6) | −0.1325 (10) | −0.0036 (5) | 0.040 (5) |
| C11 | 0.5438 (7) | −0.0161 (11) | 0.1014 (6) | 0.034 (5) |
| C12 | 0.4794 (7) | −0.0152 (10) | 0.0725 (6) | 0.032 (5) |
| C13 | 0.6648 (7) | 0.0406 (11) | 0.1551 (5) | 0.031 (5) |
| C14 | 0.6647 (7) | −0.0703 (11) | 0.1535 (6) | 0.033 (5) |
| C15 | 0.3573 (7) | 0.0415 (12) | 0.0253 (6) | 0.035 (5) |
| C16 | 0.3603 (6) | −0.0718 (12) | 0.0220 (5) | 0.029 (5) |
| C17 | 0.7987 (9) | 0.036 (2) | 0.2033 (10) | 0.101 (10) |
| C18 | 0.7894 (9) | −0.064 (2) | 0.2248 (9) | 0.090 (9) |
| C19 | 0.2475 (8) | 0.0410 (13) | −0.0221 (6) | 0.046 (6) |
| C20 | 0.2506 (8) | −0.073 (2) | −0.0260 (6) | 0.054 (7) |
| S21 | 0.6156 (2) | 0.1985 (3) | 0.3050 (2) | 0.0443 (14) |
| S22 | 0.6144 (2) | 0.4413 (3) | 0.3029 (2) | 0.0395 (14) |
| S23 | 0.4616 (2) | 0.1946 (3) | 0.2343 (2) | 0.0455 (14) |
| S24 | 0.4603 (2) | 0.4395 (3) | 0.2326 (2) | 0.0394 (13) |
| S25 | 0.7602 (2) | 0.1779 (3) | 0.3544 (2) | 0.062 (2) |
| S26 | 0.7593 (2) | 0.4676 (3) | 0.3493 (2) | 0.052 (2) |
| N21 | 0.3373 (6) | 0.1979 (10) | 0.1702 (5) | 0.047 (5) |
| N22 | 0.3355 (6) | 0.4303 (9) | 0.1668 (5) | 0.042 (5) |
| C21 | 0.5705 (7) | 0.3187 (10) | 0.2828 (6) | 0.034 (5) |
| C22 | 0.5063 (7) | 0.3171 (11) | 0.2535 (6) | 0.032 (5) |
| C23 | 0.6926 (7) | 0.2657 (12) | 0.3303 (6) | 0.042 (6) |
| C24 | 0.6920 (7) | 0.3773 (13) | 0.3278 (6) | 0.040 (6) |
| C25 | 0.3888 (7) | 0.2565 (11) | 0.1966 (6) | 0.037 (5) |
| C26 | 0.3880 (7) | 0.3726 (12) | 0.1942 (6) | 0.036 (5) |
| C27 | 0.8213 (8) | 0.2690 (13) | 0.3940 (7) | 0.062 (7) |
| C28 | 0.8307 (8) | 0.3758 (15) | 0.3556 (7) | 0.067 (7) |
| C29 | 0.2822 (8) | 0.2533 (13) | 0.1420 (7) | 0.052 (6) |
| C30 | 0.2811 (7) | 0.3700 (13) | 0.1398 (6) | 0.043 (6) |
| Cl1*A*† | 0.117 (2) | 0.145 (7) | 0.0473 (11) | 0.15 (2) |
| Cl1*B*† | 0.1196 (8) | 0.265 (3) | 0.0619 (10) | 0.212 (13) |
| Cl2 | 0.0018 (5) | 0.3436 (6) | −0.0008 (4) | 0.169 (4) |
| Cl3 | −0.0755 (3) | 0.1304 (7) | 0.0292 (3) | 0.147 (4) |
| C31*A*† | 0.030 (2) | 0.260 (3) | 0.061 (2) | 0.114 (14)‡ |
| C31*B*† | 0.031 (5) | 0.187 (9) | 0.034 (4) | 0.11 (3)‡ |
| C32*A*† | 0.075 (3) | 0.080 (4) | 0.044 (2) | 0.028 (14)‡ |
| C32*B*† | 0.012 (2) | 0.143 (3) | 0.051 (2) | 0.108 (14)‡ |

† The refined occupancy factors, 0.30 (3), for all solvent atoms with suffix *A* and for atoms with suffix *B*, 0.70 (3), were constrained to sum to 1.000. ‡ Atoms refined with isotropic displacement parameter.

Table 2. *Selected geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Tl—I1 | 2.7599 (14) | S15—C17 | 1.82 (2) |
| Tl—I3 | 2.7621 (15) | S16—C14 | 1.750 (13) |
| Tl—I2 | 2.7627 (14) | S16—C18 | 1.79 (2) |
| Tl—I4 | 2.7674 (14) | N11—C15 | 1.32 (2) |
| S1—C1 | 1.724 (13) | N11—C19 | 1.37 (2) |
| S1—C3 | 1.740 (14) | N12—C20 | 1.35 (2) |
| S2—C4 | 1.739 (14) | N12—C16 | 1.36 (2) |
| S2—C1 | 1.744 (13) | C11—C12 | 1.35 (2) |
| S3—C2 | 1.749 (13) | C13—C14 | 1.35 (2) |
| S3—C5 | 1.751 (14) | C15—C16 | 1.38 (2) |
| S4—C2 | 1.746 (13) | C17—C18 | 1.34 (2) |
| S4—C6 | 1.752 (13) | C19—C20 | 1.39 (2) |
| S5—C3 | 1.749 (14) | S21—C21 | 1.745 (13) |
| S5—C7 | 1.83 (2) | S21—C23 | 1.759 (14) |
| S6—C4 | 1.746 (14) | S22—C21 | 1.750 (13) |
| S6—C8 | 1.840 (14) | S22—C24 | 1.750 (14) |
| N1—C5 | 1.33 (2) | S23—C25 | 1.731 (14) |
| N1—C9 | 1.35 (2) | S23—C22 | 1.754 (13) |
| N2—C6 | 1.311 (15) | S24—C26 | 1.756 (14) |
| N2—C10 | 1.38 (2) | S24—C22 | 1.770 (14) |
| C1—C2 | 1.37 (2) | S25—C23 | 1.740 (15) |
| C3—C4 | 1.37 (2) | S25—C27 | 1.771 (14) |
| C5—C6 | 1.43 (2) | S26—C24 | 1.747 (15) |
| C7—C8 | 1.53 (2) | S26—C28 | 1.81 (2) |
| C9—C10 | 1.43 (2) | N21—C25 | 1.31 (2) |
| S11—C11 | 1.745 (13) | N21—C29 | 1.36 (2) |
| S11—C13 | 1.761 (13) | N22—C26 | 1.33 (2) |
| S12—C11 | 1.734 (14) | N22—C30 | 1.37 (2) |
| S12—C14 | 1.751 (13) | C21—C22 | 1.35 (2) |
| S13—C12 | 1.743 (13) | C23—C24 | 1.36 (2) |
| S13—C15 | 1.761 (14) | C25—C26 | 1.41 (2) |
| S14—C16 | 1.744 (13) | C27—C28 | 1.58 (2) |
| S14—C12 | 1.749 (13) | C29—C30 | 1.42 (2) |
| S15—C13 | 1.726 (13) | | |
| I1—Tl—I3 | 112.99 (4) | C11—C12—S14 | 121.4 (10) |
| I1—Tl—I2 | 108.73 (5) | S13—C12—S14 | 116.2 (7) |
| I1—Tl—I4 | 108.79 (4) | C14—C13—S15 | 130.3 (11) |
| I3—Tl—I2 | 106.76 (5) | C14—C13—S11 | 115.7 (10) |
| I3—Tl—I4 | 109.98 (5) | S15—C13—S11 | 114.0 (8) |
| I2—Tl—I4 | 109.53 (4) | C13—C14—S16 | 127.7 (11) |
| C1—S1—C3 | 95.9 (6) | C13—C14—S12 | 117.5 (10) |
| C4—S2—C1 | 95.5 (6) | S16—C14—S12 | 114.8 (8) |
| C2—S3—C5 | 95.1 (6) | N11—C15—C16 | 123.8 (13) |
| C2—S4—C6 | 95.8 (6) | N11—C15—S13 | 121.0 (11) |
| C3—S5—C7 | 99.8 (7) | C16—C15—S13 | 115.1 (11) |
| C4—S6—C8 | 103.6 (7) | N12—C16—C15 | 121.6 (12) |
| C5—N1—C9 | 116.9 (12) | N12—C16—S14 | 119.7 (11) |
| C6—N2—C10 | 115.3 (12) | C15—C16—S14 | 118.7 (11) |
| C2—C1—S1 | 123.6 (10) | C18—C17—S15 | 121.7 (17) |
| C2—C1—S2 | 121.2 (10) | C17—C18—S16 | 122.3 (15) |
| S1—C1—S2 | 115.2 (7) | N11—C19—C20 | 120.3 (14) |
| C1—C2—S4 | 122.0 (11) | N12—C20—C19 | 123.7 (14) |
| C1—C2—S3 | 121.3 (10) | C21—S21—C23 | 95.1 (7) |
| S4—C2—S3 | 116.8 (7) | C21—S22—C24 | 95.0 (7) |
| C4—C3—S1 | 116.7 (11) | C25—S23—C22 | 96.0 (7) |
| C4—C3—S5 | 127.2 (11) | C26—S24—C22 | 95.3 (6) |
| S1—C3—S5 | 116.0 (9) | C23—S25—C27 | 102.1 (7) |
| C3—C4—S2 | 116.6 (11) | C24—S26—C28 | 101.8 (8) |
| C3—C4—S6 | 128.9 (11) | C25—N21—C29 | 117.3 (13) |
| S2—C4—S6 | 114.5 (8) | C26—N22—C30 | 115.6 (12) |
| N1—C5—C6 | 121.8 (12) | C22—C21—S21 | 122.3 (10) |
| N1—C5—S3 | 121.4 (11) | C22—C21—S22 | 122.5 (11) |
| C6—C5—S3 | 116.8 (10) | S21—C21—S22 | 115.2 (8) |
| N2—C6—C5 | 123.2 (12) | C21—C22—S23 | 122.7 (11) |
| N2—C6—S4 | 121.4 (10) | C21—C22—S24 | 122.1 (10) |
| C5—C6—S4 | 115.4 (10) | S23—C22—S24 | 115.2 (7) |
| C8—C7—S5 | 112.2 (11) | C24—C23—S25 | 128.8 (11) |
| C7—C8—S6 | 113.5 (11) | C24—C23—S21 | 116.7 (11) |
| N1—C9—C10 | 120.6 (14) | S25—C23—S21 | 114.5 (8) |
| N2—C10—C9 | 122.3 (14) | C23—C24—S26 | 128.0 (12) |
| C11—S11—C13 | 96.4 (6) | C23—C24—S22 | 117.3 (11) |
| C11—S12—C14 | 96.2 (6) | S26—C24—S22 | 114.7 (9) |
| C12—S13—C15 | 95.6 (6) | N21—C25—C26 | 121.5 (13) |
| C16—S14—C12 | 94.3 (6) | N21—C25—S23 | 121.3 (11) |
| C13—S15—C17 | 100.5 (7) | C26—C25—S23 | 117.1 (11) |
| C14—S16—C18 | 100.7 (8) | N22—C26—C25 | 123.3 (13) |
| C15—N11—C19 | 115.9 (12) | N22—C26—S24 | 120.5 (11) |
| C20—N12—C16 | 114.7 (12) | C25—C26—S24 | 116.1 (11) |
| C12—C11—S12 | 123.6 (10) | C28—C27—S25 | 112.7 (11) |
| C12—C11—S11 | 122.3 (11) | C27—C28—S26 | 112.5 (11) |
| S12—C11—S11 | 114.2 (8) | N21—C29—C30 | 121.2 (14) |
| C11—C12—S13 | 122.4 (11) | N22—C30—C29 | 121.0 (14) |

The *UCLA* crystallographic program package (Strouse, 1985) was employed for the data reduction, structure solution and refinement.

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Lists of structure factors, anisotropic displacement parameters and least-squares-planes data have been deposited with the IUCr (Reference: SZ1040). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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# A β-Adrenergic Agonist: Protonated Terbutaline Hemisulfate

RAKHI SENGUPTA AND JIBAN K. DATTAGUPTA

*Crystallography & Molecular Biology Division, Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Calcutta-700064, India*

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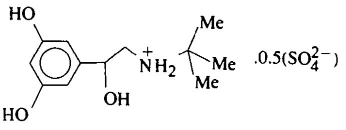
## Abstract

The title molecule, *tert*-butyl[2-(3,5-dihydroxyphenyl)-2-hydroxyethyl]ammonium hemisulfate, $C_{12}H_{20}NO_3^+.0.5(SO_4^{2-})$, consists of a phenethylamine skeleton in which the N atom is protonated. The ethylamine side chain is in an extended conformation for both molecules in the asymmetric unit. The distance of the N atom from the centre of the benzene ring is 5.1 Å. The molecules in the unit cell are stabilized by N—H···O and O—H···O hydrogen bonds.

## Comment

Compounds having a phenethylamine backbone with an OH group substituted at the *meta* position are potent β-adrenergic agonists (O'Donnell & Wanstall, 1974). Terbutaline has a structure of this type. It is a well known β-adrenergic agonist and clinically used as a bronchodilator. The three-dimensional structure of this compound has been determined and compared with those of a few similar drug molecules.

The interatomic bond lengths and angles are similar in the two molecules (*A* and *B*) of the asymmetric unit of the title compound (I) and show no significant deviation from the average model values (Herbert, 1979) obtained by averaging the bond lengths and angles in 34 similar adrenergic compounds, except in the case of the N1—C9 bond length. This N—C bond distance is 1.529 (4) Å in molecule *A* and 1.525 (4) Å in molecule *B*, compared with the average model value of 1.486 Å. All the bond lengths and angles, however, compare well with the values obtained for terbutaline hemisulfate hydrate (Hickel, Carpy, Laguerre & Leger, 1982). Similar deviation of the N—C bond length from the average model value has also been seen in some other β-adrenergic agonists like salbutamol sulfate (Leger, Goursolle, Gadret & Carpy, 1978), clenbuterol hydrochloride (Carpy, Leger & Colleter, 1980), Alupent and orciprenaline (Beale, 1972), and fenoterol hydrobromide (Dattagupta & Sengupta, 1995).



(I)

The conformation of the ethylamine side chain with respect to the benzene ring is usually described by the torsion angles C2—C1—C7—C8 ($\tau_1$) and C1—C7—C8—N ($\tau_2$). Molecule *A* has an extended conformation with $\tau_1 = -56.1\,(3)$ and $\tau_2 = 170.3\,(2)°$. The corresponding angles in molecule *B* are 127.3 (3) and −157.0 (2)°, respectively. Although the bond lengths and angles are similar, the torsion angles in the present structure differ somewhat from those in terbutaline hemisulfate hydrate (Hickel, Carpy, Laguerre & Leger, 1982) in which $\tau_1$ is 62 (1) in *A* and 59 (1)° in *B* and $\tau_2$ has a value of 182 (1) in *A* and 180 (1)° in *B*. A study of these torsion angles in other β-adrenergic agonists like salbutamol sulfate (Leger, Goursolle, Gadret & Carpy, 1978), clenbuterol hydrochloride (Carpy, Leger & Colleter, 1980), Alupent and orciprenaline (Beale, 1972), fenoterol hydrobromide (Dattagupta & Sengupta, 1995) also show that $\tau_1$ is distributed around ± 90 and $\tau_2$ around ± 180°. This indicates that a maximally extended ethylamine side chain approximately perpendicular to the benzene ring, may be the receptor preferred conformation for this class of drugs.

The distance of the amino-N atom from the centre of the benzene ring is 5.1 Å in both of the molecules in the asymmetric unit. This distance seems to be fairly constant in similar biologically active amines like *p*-hydroxyephedrine hydrochloride (Dattagupta, Pattanayek & Saha, 1981), synephrine monohydrogenphosphate monohydrate (Dattagupta, Meyer & Mukhopadhyay, 1982), L-phenylephrine hydrochloride (Bhaduri, Saha, Dattagupta & Meyer, 1983), 2,2′-di-*N*-methylamino-1,1′-di-*p*-hydroxyphenyldiethylene ether dihydrobromide (Mukhopadhyay & Dattagupta, 1988) and also in β-adrenergic agonists like salbutamol sulfate (Leger, Goursolle, Gadret & Carpy, 1978), Alupent and