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**Structure of the Conducting Salt of Pyrazinoethylenedithiotetrathiafulvalene (PEDTTTF):
 α -(PEDTTTF)₂IBr₂, at 98 K**

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Abstract. Bis{2-(dithiolo[4,5-*b*]dithiin-2-ylidene)dithiolo[4,5-*b*]pyrazinium} dibromiodide, (C₁₀H₆N₂S₆)₂·IBr₂, *M_r* = 979.86, triclinic, *P* $\bar{1}$, *a* = 8.850 (4), *b* = 5.691 (2), *c* = 15.377 (7) Å, α = 99.04 (4), β = 87.23 (4), γ = 108.35 (4)°, *V* = 726.0 Å³, *Z* = 1, *D_x* = 2.237 g cm⁻³, Mo *K* α , λ = 0.71069 Å, μ = 48.9 cm⁻¹, *F*(000) = 475, *T* = 98 K. Final *R* = 0.077 for 3879 observed reflections. Packing is similar to that of the room-temperature structure. The disorder of the ethylene group observed at room temperature (RT) has disappeared at 98 K. The planarity of the tetrathiafulvalene moiety is better in the low-temperature (LT) structure with the greatest deviation from the mean plane of this moiety being

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Table 1. Positional ($\times 10^4$) and equivalent isotropic thermal parameters for the non-H atoms with e.s.d.'s in parentheses

$$B_{eq} = \frac{1}{3} \pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	$B_{eq}(\text{\AA}^2)$
I1	0	0	0	0.9
Br	-2256 (1)	2271 (1)	138.3 (5)	1.3
S1	2370 (2)	2178 (2)	6308 (1)	0.9
S2	4756 (2)	7117 (2)	6325 (1)	0.9
S3	930 (2)	2605 (3)	4505 (1)	0.9
S4	3293 (2)	7665 (2)	4506 (1)	0.9
S5	3298 (2)	1298 (3)	7999 (1)	1.1
S6	6308 (2)	7117 (3)	7974 (1)	1.0
N1	-243 (6)	3121 (10)	2992 (3)	1.1
N2	1986 (6)	7909 (9)	2996 (3)	1.0
C1	3181 (7)	4781 (11)	5780 (4)	1.0
C2	2555 (6)	4989 (10)	5008 (4)	0.8
C3	3670 (6)	3252 (10)	7206 (4)	0.8
C4	4809 (6)	5541 (10)	7205 (4)	0.8
C5	834 (6)	4169 (10)	3622 (4)	0.8
C6	1938 (6)	6546 (10)	3622 (4)	0.8
C7	5097 (7)	2647 (11)	8653 (4)	1.0
C8	5575 (7)	5481 (11)	8896 (4)	1.2
C9	-201 (7)	4465 (12)	2348 (4)	1.2
C10	891 (7)	6843 (12)	2357 (4)	1.2

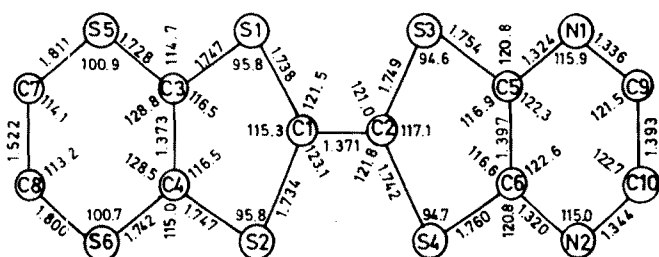


Fig. 1. Atom-numbering scheme of the donor with bond distances (\AA) and angles ($^\circ$). E.s.d.'s are 0.005–0.008 \AA for distances and 0.03–0.06 $^\circ$ for angles.

0.037 (7) \AA in the LT and 0.049 (6) \AA in the RT structure for C(3) in both cases. There is no dimerization of the donor molecules in the stacking direction since the distances of the mean planes of the tetra-thiafulvalene moiety are 3.452 (7) \AA within and 3.481 (7) \AA between the dimers and the difference of 0.029 (7) \AA is not significant. There is no such dimerization in the RT structure either with the corresponding distances being 3.588 (6) and 3.592 (6) \AA . There is significant shortening in the LT structure of the S...S and S...N contacts by as much as 0.09 \AA .

Experimental. Title compound prepared according to literature (Terzis, Psycharis, Hountas & Papavassiliou, 1988). Crystal was a hexagonal plate 0.3 \times 0.3 \times 0.1 mm. Intensity data collected on Rigaku automated four-circle diffractometer. Lattice parameters from 20 reflections in the range $20 < 2\theta < 35^\circ$. Data with $2\theta \leq 60^\circ$ (range of $hkl = 0 \rightarrow 12, -7 \rightarrow 7, -21 \rightarrow 21$), $\theta/2\theta$

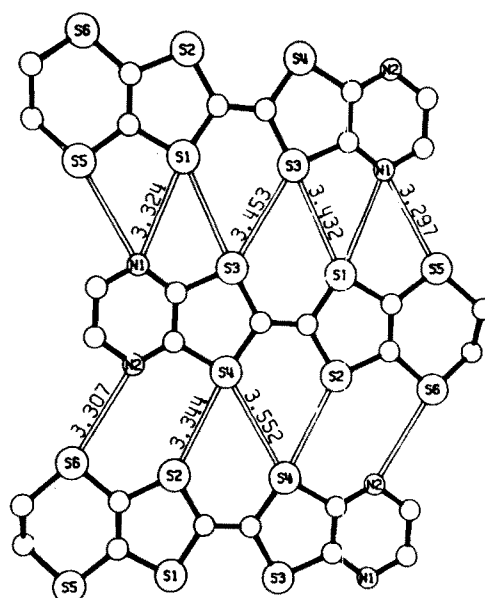


Fig. 2. Intrastack S...S and S...N contacts (\AA). E.s.d.'s are 0.003–0.005 \AA .

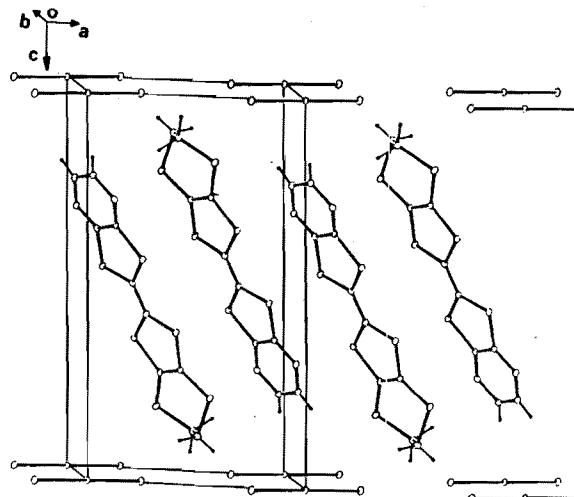


Fig. 3. An ORTEP packing diagram (Johnson, 1976).

scan mode, scan speed $8^\circ(2\theta) \text{ min}^{-1}$, scan width $1.044^\circ + 0.5^\circ \tan\theta$. Three reflections monitored periodically showed $< 3\%$ intensity fluctuations. Lorentz and polarization but no absorption correction applied. Data collected/unique/ R_{int} /observed [$F_o \geq 3\sigma(F_o)$], 4526/4395/0.030/3879. Positions for I and Br deduced from Patterson map, remainder from difference map. Full-matrix refinement based on F with UNICSIII (Sakurai & Kobayashi, 1979) using the weighting scheme $w = (10.0 + 0.01|F_o|^2)^{-1}$ for $|F_o| < 15.0$ and $w = (\sigma^2 + 0.01|F_o|^2)^{-1}$ for $|F_o| \geq 15.0$, 196 parameters refined including the H positions. Refinement converged to: $R = 0.077$, $wR = 0.074$, $S = 0.6248$, $|\Delta/\sigma|_{\max}$

$= 0.18$, $\Delta\rho_{\max}/\Delta\rho_{\min} = 0.6/-0.6 \text{ e } \text{\AA}^{-3}$. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). The final atomic parameters are given in Table 1,* bond lengths and angles in Fig. 1, the intrastack S...S and S...N contacts in Fig. 2, and the packing arrangement in Fig. 3.

* Lists of observed and calculated structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51508 (42 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related literature. The room-temperature structure is reported in Terzis *et al.* (1988).

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