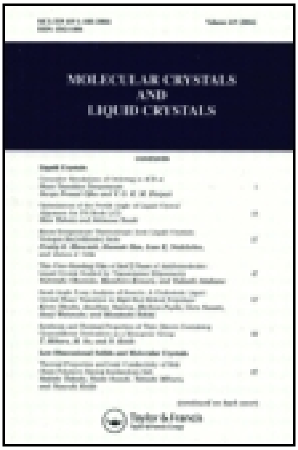

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2-Fluoro-5,6,11,12-Tetraselenotetracene-Br, Metallic Down to at Least 2K?

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2-FLUORO-5,6,11,12-TETRASELENOTETRACENE-$BR_{0.5}$, *METALLIC DOWN TO AT LEAST 2K ?*

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Abstract. The 2-FTSeT-$Br_{0.5}$ complex [(2-Fluoro-5,6,11,12-tetraselenotetracene)-$Br_{0.5}$] has been prepared by electrocrystallisation. Its crystal structure is presented together with conductivity and susceptibility data. Introduction of a fluorine substituent in the 2-position appears to suppress the phase transitions observed in the parent TSeT-$halogen_{0.5}$ compounds

PREPARATION.

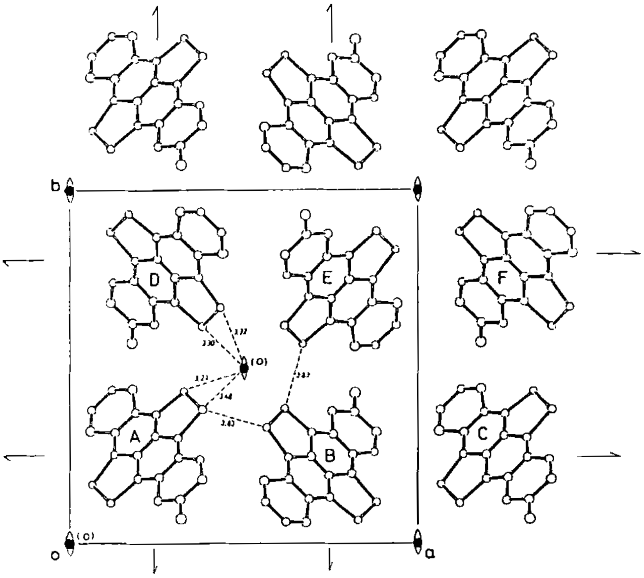
The 2-FTSeT-$Br_{0.5}$ complex has been prepared by electrocrystallisation at a Pt-anode in a DMF-chlorobenzene mixture (20 : 80) with tetrabutylammonium-bromide as supporting electrolyte ($I=1\mu A/cm^2$). Crystals obtained were of the approximate size 7 x 0.03 x 0.03 mm.

CRYSTAL STRUCTURE.

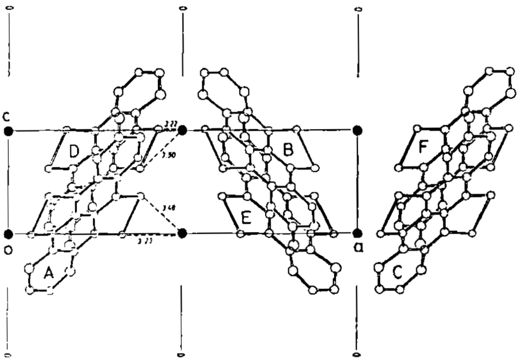
As seen from the table, 2-FTSeT-$Br_{0.5}$ crystallizes in the crystal system of the TSeT-$I_{0.5}$ and not in that one of the parent compound TSeT-$Br_{0.5}$ (1, 2).
At least 85 % of the fluorine substituents are on the sites indicated in figure 1 and figure 2. It is not clear yet by wich influence of the fluorine substituent this relatively high degree of order of the structure is achieved. Noteworthy is also the exceptionally short interplanar distance of 3.30 Å between adjacent 2-FTSeT-molecules.

TABLE Comparison of crystal data.

	FTSeT-$Br_{0.5}$	TSeT-$I_{0.5}$	TSeT-$Br_{0.5}$
Crystal system	orthorhombic	orthorhombic	monoclinic
Space group	$P_{2_1 2_1 2}$	$P_{2_1 2_1 2}$	$P_{2/n}$
Site symmetry of the Donor	C_1	C_1	C_1
Se-Se interstack	3,83	3,76	3,86
Se-Se intrastack	3,46	3,45	3,49 / 3,50
Interplanar distance	3,30	3,40	3,42 / 3,45
Se-X distance	3,23 3,48 3,22 3,50	3,42 3,71 3,42 3,50	3,14 3,56 3,14 3,55
a	17,655	18,366	17,686
b	17,661	17,450	5,083
c	5,125	5,077	17,688
∢ long molecular axis vs. stacking axis	40°	42°	42° / 42°
∢ short molecular axis vs. stacking axis	90°	88°	87° / 86°
ρ_{RT} (Ωcm)	6×10^{-4}	5×10^{-4}	5×10^{-4}



Projection of the crystal structure on the (a,b) plane



Projection of the crystal structure on the (a,c) plane

FIGURE 1 and FIGURE 2

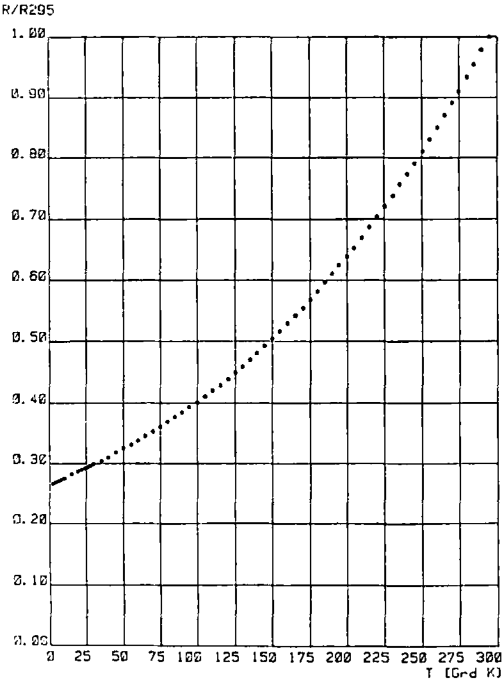


FIGURE 3

SPECIFIC ELECTRICAL RESISTANCE OF
$(FTSeT)_2Br$
NORMALIZED TO 295 K AS A FUNCTION
OF TEMPERATURE

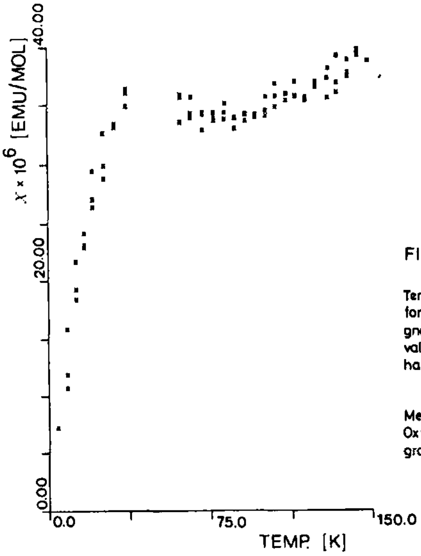


FIGURE 4

Temperature dependence of the residual static susceptibility for FTSeT-$Br_{0,5}$ after substraction of the constant core diamagnetic susceptibility, taken from the mean of the measured value for FTSeT (-229,4 ±30·10^{-6} emu/mol 260K>T>150K) plus half of the Pascal value for Br (-30,6/2·10^{-6} emu/mol).

Measurements were performed on a Faraday balance from Oxford Instruments at 66.02 kG and three different field gradients (300, 500, 700 G/cm) on samples of 10 to 16 mg.

PHYSICAL PROPERTIES.

2-FTSeT-$Br_{0.5}$ does not show any indication of a phase transition as shown by the electrical resistivity measurements (down to 2 K), figure 3. The almost constant value of the magnetic susceptibility in the temperature range 150 K to 35 K corresponds roughly to the behaviour observed in the TSeT-$Br_{0.5}$. The drop of the susceptibility below 35 K however does suggest a phase transition which did not show up in the el. resistivity measurements (figure 4)!

CONCLUDING REMARKS.

We do not know yet to what extent the remaining disorder (15%) is responsible for the stabilization of the metallic state. Works to clarify the electronic influence(e.g. change of the degree of charge transfer) induced by the substituent in fully ordered structures will be of particular interest.

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