A new crystal structure for $(BEDT–TTF)_2SbF_6$ and some of its physical properties

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Abstract. A new crystal structure for *bis*(ethylenedithio)tetrathiafulvalene [$(BEDT–TTF)_2SbF_6$] was determined by single crystal X-ray diffraction. The crystal structure was refined in the $P\bar{1}$ space group at room temperature. Crystal data for new structure are as follows: triclinic, $a = 8{\cdot}670$ (2) Å, $b = 8{\cdot}664$ (2) Å, $c = 16{\cdot}842$ (5) Å, $\alpha = 89°{\cdot}29$ (2), $\beta = 90°{\cdot}71$ (3), $\gamma = 92°{\cdot}67$ (1), $V = 1263{\cdot}64$ Å^3, $Z = 2$, $D_x = 2{\cdot}136$ g cm^{-3}, (Mo–Kα), $\lambda = 0{\cdot}7107$ Å, $R = 0{\cdot}057$ for a total of 5517 independent reflections. The donors form a trimerized column, and the band structure calculated by the tight-binding approximation shows band insulator properties. The temperature dependent of the d.c. resistivity shows a semiconducting behaviour with room temperature resistivity along the *c*-axis; $\rho_{290\,K} = 5{\cdot}6$ ohm cm.

Keywords. Organic conductors; β-$(ET)_2PF_6$; $(ET_2)SbF_6$; electrocrystallization.