E1 – 09

Structural and some physical properties of (BEDT-TTF)3(SbF6)2

Organic conductors of BEDT-TTF compounds (BEDT-TTF; Bisethylene dithiotetrahiafulvlene) have been studied extensively because of their potential designability as superconducting materials. One of the characteristic features of BEDT-TTF salts is the ability to exhibit a large number of crystal types and polymorphism from the same anion and solvent. The room temperature crystal structures has been reported for (BEDT- TTF) $_2SbF_6$, monoclinic space group I2/c with a = 33.56 Å, b = 0.6.70 Å, c = 14.4 Å, (β = 90.71 Å. In this, we report a new crystal structural data of the Sb F_6 complex and some of its physical properties.

Titled compound crystals are prepared by the electrolytic oxidation of BEDT-TTF in 1,1,2,-tricloroethane as the solvent with (n—Bu4n0SbF6 as the salt. X-ray unit cell determination and data collection is performed and final unit cell parameters are determined by the refinement of 5517 reflections. Temperature dependence of the electrical resistivity is measured over the range 220-350 K< on a single crystal by using the standard four-probe technique. Overlap integrals of the HOMO and the band structure are calculated.

Crystal data for new structure are Triclinic, PI, a = 8.670 (2) Å b = 8.664 (2) Å, c = 16.842 (5) Å, (a = 89^o .29,(β = 90^o .71 (3), (γ = 92^o.67 (1) V = 1263.64 Å^3, Z = 2, D_x = 2.136 g cm^{-3}

The final R = 0.057 for total 5517 independent reflections. The donors from a trimerized columm, and the band structure calculated by the tightbinding approximation shows a band insulator. The temperature dependence of the d.c. resistivity shows a

semiconducting behaviour with room temperature resistivity along the c-axis; p_{290k}=5.6 ohm cm and the activation energy is 0.25 eV. In contrast to the previously reported SbF6 salt having the 2:1 composition the present salt has 3:2 composition.

The type of the present structure is an entirely new and which has no analog among the reported BEDT-TTF salts.