Structure and Phase Transition in $(C_2H_5NH_3)_3Sb_2Cl_9 \cdot (C_2H_5NH_3)SbCl_4$; X-ray, DSC and Dielectric Studies

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The structure of $(C_2H_5NH_3)_3Sb_2Cl_9 \cdot (C_2H_5NH_3)SbCl_4$ at 295 K has been determined. The crystals are orthorhombic, space group $Pna2_1$ (a = 16.925(3), b = 24.703(5), c = 7.956(2) Å, V = 3326.4(12) Å^3, Z = 4, d_c = 2.018, d_m = 2.01(1) Mg m^{-3}). They consist of an anionic sublattice composed of two different polymeric zig-zag chains. One is built of $Sb_2Cl_9^{3-}$ units (corner sharing octahedra) and the other one is made of corner sharing $SbCl_5^{2-}$ square pyramids. In the cavites between the polyanionic chains four non-equivalent ethylammonium cations are located. Three of them are disordered. The cations are connected to the anions by weak N-H...Cl hydrogen bonds. A first order phase transition of the order-disorder type was found at 274 K. It was studied by DSC, dielectric and X-ray diffraction methods. The mechanism of the phase transition is attributed to the ordering of at least one of the ethylammonium cations.

Key words: Ethylamine; Chloroantimonate(III); Structure; Phase Transition.