

# Phase Transitions Mechanism and Distortion of $\text{SbCl}_6^{3-}$ Octahedra in Bis(*n*-butylammonium) Pentachloroantimonate(III) $(\text{C}_4\text{H}_9\text{NH}_3)_2[\text{SbCl}_5]$

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Bis(*n*-butylammonium) pentachloroantimonate(III) was obtained in a reaction of *n*-butylammonium chloride and antimony trichloride (molar ratio 2 : 1; cation : Sb) in acidic aqueous solution. To obtain further information about the mechanism of the earlier reported phase transitions at 229 and 315 K the structure was determined at 100, 260 and 340 K. The orthorhombic system was found in all phases, space groups *Ibam* at 340 K and *Pccn* at 260 and 100 K. In all phases the anionic sublattice consists of  $[\text{SbCl}_6]^{3-}$  octahedra, connected *via cis* chlorine atoms, forming one-dimensional zig-zag  $\{[\text{SbCl}_5]^{2-}\}_n$  chains extended along the *c* direction. The *n*-butylammonium cations are located between the inorganic chains, with  $-\text{NH}_3^+$  groups facing the oppositely charged polyanions. The phase transitions are of the order-disorder type. They are related to changes in molecular dynamics of the *n*-butylammonium cations. At high temperature the cations reorient, on decreasing temperature the reorientations are successfully frozen. This leads to the formation of N-H...Cl hydrogen bonds, which significantly deform the octahedral coordination of the Sb atoms.

*Key words:* Chloroantimonates(III), *n*-Butylammonium Cation, Phase Transition, Disorder