

Phase Transitions and Distortion of $[\text{BiCl}_6]^{3-}$ Octahedra in $(\text{C}_3\text{H}_5\text{NH}_3)_3[\text{BiCl}_6]$ – DSC and Single-Crystal X-Ray Diffraction Studies

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The DSC diagram of tris(allylammonium) hexachlorobismuthate(III), $(\text{C}_3\text{H}_5\text{NH}_3)_3[\text{BiCl}_6]$, revealed three anomalies at 152, 191 and 299 K. The structure of the salt was determined at 200 and 315 K, below and above the high-temperature phase transition at 299 K. In both phases the crystals are monoclinic. At 200 K the space group is $C2/c$ whereas at 315 K it is $C2/m$. The structures, at both temperatures, are composed of $[\text{BiCl}_6]^{3-}$ octahedra and allylammonium cations. The organic and inorganic moieties are attracted to each other by a network of the N–H...Cl hydrogen bonds. The relationship between corresponding parameters of the unit cells has been found. The phase transition at 299 K, of the order-disorder type, is attributed to the ordering of one non-equivalent allylammonium cation in the low-temperature phase.

Key words: Chlorobismuthates(III), Allylammonium Cation, Phase Transition, Disorder, Octahedral Distortion