

The structure, phase transition and molecular dynamics of $[\text{C}(\text{NH}_2)_3]_3[\text{Sb}_2\text{Br}_9]$.

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The crystal structures of $[\text{C}(\text{NH}_2)_3]_3[\text{Sb}_2\text{Br}_9]$ ($\text{Gu}_3\text{Sb}_2\text{Br}_9$) at 300 K and of $[\text{C}(\text{NH}_2)_3]_3[\text{Sb}_2\text{Cl}_9]$ ($\text{Gu}_3\text{Sb}_2\text{Cl}_9$) at 90 and 300 K are determined. The compounds crystallize in the monoclinic space group: $C 2/c$. The structure is composed of $\text{Sb}_2\text{X}_9^{3-}$ ($X = \text{Cl}, \text{Br}$) ions, which form two-dimensional layers through the crystal, and guanidinium cations. In $\text{Gu}_3\text{Sb}_2\text{Br}_9$ the structural phase transformation of the first-order type is detected at 435/450 K (on cooling/heating) by the DSC and dilatometric techniques. The dielectric relaxation process in the frequency range between 75 kHz and 5 MHz over the low temperature phase indicates reorientations of weakly distorted guanidinium cations. The proton ^1H NMR second-moment and spin-lattice relaxation time, T_1 , temperature runs for the polycrystalline $\text{Gu}_3\text{Sb}_2\text{Br}_9$ sample indicate a complex cation motion. A significant dynamical non-equivalence of two guanidinium cations was found. The possible mechanism of the phase transition in $\text{Gu}_3\text{Sb}_2\text{Br}_9$ is discussed on the basis of the results presented.

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