Structure-property relationships in hybrid $(C_3H_5N_2)_3[Sb_2I_9]$ and $(C_3H_5N_2)_3[Bi_2I_9]$ isomorphs.

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Streszczenie

Two hybrid crystals imidazolium iodoantimonate(III) and iodobismuthate(III), $(C_3H_5N_2)_3[Sb_2I_9]$ (ImIA) and $(C_3H_5N_2)_3[Bi_2I_9]$ (ImIB), have been synthesized and characterized in a wide temperature range (100–350 K) by means of X-ray diffraction, dielectric spectroscopy, proton magnetic resonance (^{1}H NMR), FT-IR spectroscopy and optical observations. They undergo two temperature induced solid–solid structural phase transitions. The first one, quasi-continuous (with temperature hysteresis below 1 K), occurs at 324 K in ImIA and 327 K in ImIB, and the second one, clearly of the first order, at 273/278 (cooling/heating) and 291/295 K, in ImIA and ImIB, respectively. Ferroelastic properties are maintained in low-temperature phases. Both materials are isomorphic in the corresponding phases. High temperature phase I has a hexagonal $P6_3/mmc$ symmetry, and phase II has orthorhombic $Cmcm$. The crystal architecture is composed of discrete, face-sharing bioctahedra $[M_2I_9]^{3-}$ (M: Sb, Bi) and imidazolium cations which are highly disordered over phases I and II. The dynamics of the imidazolium cations has a prominent impact on the stability of the particular phases.

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