Unprecedented solid-state chemical reaction—from $(C_3N_2H_5)_3SbBr_6{\cdot}H_2O$ to $(C_3N_2H_5)_5Sb_2Br_{11}$. From centrosymmetric to non-centrosymmetric crystal structure.

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Streszczenie

Tris(imidazolium) hexabromoantimonate(III) hydrate, (C3N2H5)3SbBr6·H2O, (abbreviated as TIBA) has been synthesized and characterized by X-ray (at 295, 225, 160, and 110K), differential scanning calorimetry, dilatometry, and dielectric spectroscopy. At room temperature (phase I), the structure consists of discrete SbB_6^{-} anions, disordered imidazolium cations, and water molecules forming a 3D array of hydrogen bonds. Below room temperature, TIBA was found to undergo isostructural discontinuous phase transition at 212/221K (cooling–heating) (P21/c↔P21/c). The phase transition mechanism is characterized by two contributions: an order–disorder (cationic substructure) and a displacive (water molecules) one. At high temperatures, the TIBA crystal was found to undergo an unprecedented in situ solid-state chemical reaction:

(1)2(C3N2H5)3SbBr6·H2O(S)→(C3N2H5)5Sb2Br11(S)+(C3N2H5)Br(S)+2H2OThis chemical transformation leads to multiphase crystallites dominated by an amorphous phase of (C3N2H5)5Sb2Br11. The creation of ferroelectric crystallites – (C3N2H5)5Sb2Br11 – in an “annealed” sample of (C3N2H5)3SbBr6·H2O was confirmed by X-ray diffraction phase analysis, dielectric spectroscopy, and pyroelectric measurements. The dielectric response of the electric permittivity and the critical slowing down of the process observed near 140K in the “annealed” sample of TIBA are treated as a “fingerprint” of a neat (C3N2H5)5Sb2Br11 ferroelectric.

Słowa kluczowe

Halogenoantimonates(III), phase transition, hydrogen bonds, Ferroelectric hybridmaterials

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