Structural characterization, thermal and electric properties of imidazolium bromoantimonate(III): $[C_3H_5N_2]_3[Sb_2Br_9]$.

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Streszczenie

Tris(imidazolium) nonabromodiantimonate(III), , is trimorphic. Its crystal structure has been determined at 100 K (form I) and 293 K (form II) by X-ray single crystal diffraction in, respectively, the monoclinic space groups, (form I) and (form II). In both structures, the anionic sublattice forms corrugated two-dimensional layers in the plane. In forms I and II there are, respectively, three and two crystallographically independent imidazolium cations. Two types of cations are present in the structures: the one that occupies cavities within the polyanions layer appears to be ordered in the lowest temperature form I and disordered in form II. The second type of imidazolium cations placed between the layers is ordered over the studied temperature region. The temperature dependence of the lattice parameters has been determined between 100 and 280 K. DSC studies indicate a presence of two reversible phase transitions: continuous at 237 K and discontinuous at 373/351 K (heating–cooling) from form II to form III. The phase transition is accompanied by a huge entropy transition () equal to ca. , which suggests an order (form II)–disorder (form III) transition mechanism. The dielectric relaxation process was found to appear in a low frequency region over the form I with an activation energy ca. 16.5 kJ/mol. A polydispersive character of the dielectric dispersion indicates a presence of complex molecular motions of dipolar groups in the title compound. The explanation of mechanism of the phase transition in is proposed. Projection of the crystal structure of $[C_3H_5N_2]_2[Sb_2Br_9]$ at 100 K (form I) on the cb plane as a polyhedral representation.

Słowa kluczowe

Halogenoantimonates(III), Imidazolium cation, Phase transition, Dielectric relaxation