Hybrid organic-inorganic bismuth(III)-based material $[4\text{-}NH_2C_5H_4NH]_7[BiCl_6]_2Cl$. Crystal structure, dielectric properties and molecular motions of 4-aminopyridinium cations.

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Streszczenie

4-aminopyridinium analogue, $[4\text{-}NH_2PyH]_7[BiCl_6]_2Cl$, has been synthesized and characterized by single-crystal X-ray diffraction at 100K, calorimetric, dilatometric and dielectric studies. The crystal structure is centrosymmetric with the monoclinic space group, $P2_1/n$. It consists of two discrete $[BiCl_6]^{3-}$ octahedra, one loose Cl^- anion and seven, partially disordered, 4-aminopyridinium cations. The compound reveals a reversible first-order phase transition (I→II) at 305/304K of the 'order-disorder' type. The dielectric studies disclosed a relaxation process in the kilohertz frequency region, assigned to the dynamics of organic cations, described well by the Cole-Cole relation. The ^1H NMR spin–lattice relaxation time measurements indicate a complex cations motion over the Phase II. The possible mechanism of the I → II phase transition in $[4\text{-}NH_2PyH]_7[BiCl_6]_2Cl$ is discussed.

Słowa kluczowe

Single-crystal X-ray diffraction, 1H NMR, phase transition, 4-Aminopyridium cations, Bismuthate(III)

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