Investigation of structure-properties relationship in a novel family of halogenoantimonates(III) and halogenobismuthates(III) with morpholinium cation: $[NH_2(C_2H_4)_2O]MX_4$. Crystal structure, phase transitions and dynamics of molecules.

Autorzy

Magdalena T. Owczarek

Ryszard Jakubas

Adam Pietraszko

Wojciech Medycki

Jan Baran

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Streszczenie

Three new organic-inorganic hybrids based on halogenoantimonates(III) and halogenobismuthates(III) with the morpholinium cation, [NH2(C2H4)2O]SbCl4, [NH2(C2H4)2O]SbBr4 and [NH2(C2H4)2O]BiBr4, have been prepared and characterized with DSC, TGA, DTA and single-crystal X-ray diffraction. The common feature of the crystal structures of the studied compounds is the presence of polyanionic ([MX4]∞(-)) and morpholinium (head-to-tail configuration) chains, which expand themselves parallel to each other. The antimonate derivatives are isomorphous, crystallizing in a centrosymmetric orthorhombic Pbca space group and show no phase transitions (PTs) between 110 and 370 K. On the other hand, [NH2(C2H4)2O]BiBr4 undergoes two first-order structural PTs: I ↔ II at 321/343 K (cooling/heating) and II ↔ III at 285/289 K (cooling/heating). The mechanism of the PTs is discussed on the basis of crystallographic data and (1)H NMR and infrared spectroscopy. The PT at 343 K is accompanied by a spectacular switching of the spin-lattice T1 relaxation pathway. Structural parameters analysis has been performed to discuss a structure-properties relationship.

Adres publiczny

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