Temperature-stimulus responsive ferroelastic molecular–ionic crystal: $(C_8H_{20}N)[BF_4]$.

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Streszczenie

Molecular–ionic crystals, which are built of organic cations and discrete anionic components with AMX_4 stoichiometry, easily induce structural order–disorder transitions. These phenomena can generate interesting ferroic properties. Herein, we have synthesized and characterized a novel AMX_4-type crystal, $(C_8H_{20}N)[BF_4]$ (**1**). Thermal analysis, (DSC, TGA) indicates one structural phase transition (PT) at 257/259 K (cooling/heating, I ↔ II). The structure of **1** has been solved at two temperatures, 120 and 298 K, with single-crystal X-ray diffraction. The high-temperature phase I (**1-HT**) shows a tetragonal structure with the space group *I*4/*mmm*, whereas the low-temperature phase II (**1-LT**) is monoclinic with the space group $P2_1/a$. The PT belongs, thus, to the improper ferroelastic species 4/*mmmF*2/*m* with a 4-fold multiplication of the unit cell. All four possible ferroelastic domains of phase II have been identified in polarized light microscopy. The monoclinic deformation has been shown to give rise to a characteristic parquet-like texture preserving integrity of **1**. The molecular mechanism of PT involving changes in the cationic and anionic dynamics has been postulated based on measurements of the ^1H and ^{19}F NMR spin–lattice relaxation times, T_1, and second-moment, M_2, and of the dielectric responses. The ac and dc conductivity measurements have been used to determine the transport properties of the charge carriers in **1**. The intrinsic features of molecular–ionic crystals, such as the dynamics of molecular motions, structural instability with a lattice-symmetry change, formation of domain patterns, etc., provide a crystal with unique ferroelastic properties. This type of crystal may be useful as an functional material.

Słowa kluczowe

Crystals, Insulators, Anions, Electrical conductivity, Cations

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