

Ferroelectricity and ferroelasticity in organic inorganic hybrid (Pyrrolidinium)₃[Sb₂Cl₉].

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Streszczenie

Perovskite-like materials exhibit desirable photophysical and electric properties that make them suitable for a remarkable breadth of applications in electronics and physics. In this contribution, we report on the multiphase ferroelectric and ferroelastic phenomena in a pyrrolidinium-based hybrid metal-organic material: (C₄H₈NH₂)₃[Sb₂Cl₉]. The title compound is the first pyrrolidinium derivative within the halobismuthates(III) and haloantimonates(III) families that is featured by the ferroelectric property. From a structural point of view, the crystal structure is built of [Sb₂Cl₉]³⁻ perovskite-like layers, interdigitated by layers of pyrrolidinium cations. The rich solid-state dynamics of pyrrolidinium cations endowed (C₄H₈NH₂)₃[Sb₂Cl₉] with a complex sequence of temperature-dependent phase transitions. Remarkably, polar properties have been found to occur in all six phases, including room-temperature Phase I. Insights from variable-temperature single-crystal X-ray diffraction, dielectric spectroscopy, and T₁ spin-lattice relaxation measurements revealed the general mechanism of most phase transitions, as related to the progressive ordering of nonequivalent pyrrolidinium cations. Noncentrosymmetry is probed by room-temperature second harmonic generation (SHG), while the ferroelectric property was evidenced through *P*(*E*) and dielectric measurements. The experimental values of spontaneous polarization were justified and analyzed in the context of theoretical values derived from quantum-chemical calculations. Optical measurements show that the integrity of the sample survives all of the phase transitions, despite sometimes significant deformations of the unit cell. The changes of symmetry associated with structural phase transitions are accompanied by an intriguing evolution of the ferroelastic domain structure with temperature.

Adres publiczny

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