

Ferroelectricity in ethylammonium bismuth-based organic–inorganic hybrid: (C₂H₅NH₃)₂[BiBr₅].

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Rok wydania

2020

Czasopismo

Inorganic Chemistry

Numer woluminu

59

Strony

3417-3427

DOI

10.1021/acs.inorgchem.9b03193

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The (C₂H₅NH₃)₂[BiBr₅] (EBB) crystals adopt the one-dimensional (1D) polymeric anionic form [BiBr₅]^{∞2-}, which is preferred by halobismuthates(III) exhibiting polar properties and realized in R₂MX₅ stoichiometry. Differential scanning calorimetry and dilatometric measurements reveal reversible structural phase transitions: at 160 K (phase I → phase II) and 120 K (phase II → phase III). The resolved crystal structures of EBB show the centrosymmetric space group in phase I (Aeam), polar (Pca21) in phase II, and polar (Aea2) in phase III. The presence of dielectric hysteresis loops in phases II and III evidence ferroelectric properties. The dielectric response [ε* (ω,T)] of EBB close to 160 K is characteristic of ferroelectrics with a critical slowing down process. The molecular mechanism of a paraelectric-ferroelectric phase transition at 160 K is explained as "order-disorder" (assigned to the dynamics of the ethylammonium cations) and dominating "displacive" (related to strong distortion of the 1D anionic network). The optical band gap obtained from UV-vis measurements is about 2.6 eV. The conduction band minimum is formed by the hybridized Bi 6p and Br 4p states. An analysis of the CSD results for haloantimonates(III) and halobismuthates(III) ferroelectrics characterized by [MX₄]⁻, [M₂X₉]³⁻, [MX₅]²⁻, and [M₂X₁₁]⁵⁻ anions is given.

Słowa kluczowe

Amines, Insulators, Phase transitions, Cations, Polarization

Adres publiczny

<http://dx.doi.org/10.1021/acs.inorgchem.9b03193>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>

