Structural characterization, thermal, dielectric, vibrational properties and molecular motions in $[C_3N_2H_5]_6[Bi_4Br_{18}]$.

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Streszczenie

$[C_3N_2H_5]_6[Bi_4Br_{18}]$has been synthesized and characterized by the X-ray (at 293 and 110 K), calorimetric, dilatometric and dielectric measurements. At room temperature it crystallizes in the monoclinic space group, *C*2/*m*. A crystal structure consists of disordered imidazolium cations and ordered discrete tetramers of $[Bi_4Br_{18}]^{6-}$. This compound reveals a rich polymorphism in a solid state. It undergoes three solid–solid phase transitions: from phase I to II at 426/423 K (heating–cooling), at 227 K and at 219.5/219 K. A clear dielectric relaxation process is found in the room temperature phase **II**. Infrared studies of the polycrystalline$[C_3N_2H_5]_6[Bi_4Br_{18}]$ showed that the , (ring) and modes of the imidazolium cations appeared to be very sensitive to the phase transition. ^{1}H NMR measurements confirmed a key role of the imidazolium cations in the phase transitions mechanisms at low temperatures.

Słowa kluczowe

Imidazolium, Bismuthate(III), Phase transition, Dielectric relaxation, Infrared, 1H NMR

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