Structure and phase transitions in guanidinium halogenobismuthates(III).

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Streszczenie

Differential scanning calorimetry (DSC), dilatometric and dielectric measurements have been used to study the phase transitions in $[C(NH_2)_3]_3BiBr_6$. The $[C(NH_2)_3]_3BiBr_6$ crystal undergoes four phase transitions: at 419, 429, 475 and 495 K (on heating). The high-temperature phase transition is clearly of first-order type and its high entropy effect allows classifying it as of the order–disorder type. X-ray diffraction studies showed that $[C(NH_2)_3]_3BiBr_6$ crystallises in monoclinic, centrosymmetric space group, *C*2/*c*. The anionic sublattice is composed of isolated $BiBr_6^{3-}$ octahedra. The infrared between 100 and 350 K and Raman spectra at room temperature in the frequency range related to the internal vibrations of guanidinium cations were studied for $[C(NH_2)_3]_3BiBr_6$, $[C(NH_2)_3]_3Bi_2Br_9$, $[C(NH_2)_3]_3BiCl_6xCl_2$ and $C(NH_2)_3Cl$ to analyse the dynamical state of cations. At room temperature, the cations in the studied guanidinium halogenobismuthates(III) are almost rigid, so the mechanism of high-temperature phase transitions is probably connected with the release of rotation of the cations.

Słowa kluczowe

Guanidinium halogenobismuthates(III), Infrared, Raman, DSC, Dilatometry, Phase transition

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