$(C_3N_2H_5)_3Sb_2I_9$ and $(C_3N_2H_5)_3Bi_2I_9$: ferroelastic lead-free hybrid perovskite-like materials as potential semiconducting absorbers

Autorzy

Przemysław Szklarz

Ryszard Jakubas

Wojciech Medycki

Anna Gągor

Jakub Cichos

Mirosław Karbowiak

Grażyna Bator

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Streszczenie

We have synthesised and characterised novel organic–inorganic hybrid crystals: **$(C_3N_2H_5)_3Sb_2I_9$** and **$(C_3N_2H_5)_3Bi_2I_9$** (**PSI** and **PBI**). The thermal DSC and TG analyses indicate four structural phase transitions (PTs) at 366.2/366.8, 274.6/275.4, 233.3/233.3 and 142.8/143.1 K (on cooling/heating) for **PSI** and two reversible PTs at 365.2/370.8 and 252.6/257.9 K for **PBI**. Both analogues crystallize at room temperature in the orthorhombic *Cmcm* structure, which transforms, in the case of **PBI**, to monoclinic $P2_1/n$ at low temperature. According to the X-ray diffraction results, the anionic component is discrete and built of face-sharing bioctahedra, $[M_2I_9]^{3-}$, in both compounds, whereas cations exhibit distinct dynamical disorder over high temperature phases. Dielectric spectroscopy and ^1H NMR spectroscopy have been used to characterise the dynamical state of the **$C_3N_2H_5^+$** cations. The ferroelastic domain structure has been characterised by observations under a polarized optical microscope. Both compounds are semiconductors with narrow bandgaps of 1.97 eV (**PBI**) and 2.10 eV (**PSI**).

Adres publiczny

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