



Structural characterization and properties of bis (1,4-H₂-1,2,4-triazolium) pentachlorobismuthate (III) and cocrystal of ammonium chloride with tris (1,4-H₂-1,2,4-triazolium) hexachlorobismuthate (III).

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Streszczenie

The crystal structure of two novel 1,2,4-triazolium analogues: (**TBC**) and (**TCBA**), isolated from one system, has been determined. The structure of **TCBA** is built up from cationic substructures consisting of 1,2,4-triazolium and ammonium cations, , and discrete octahedral anions. The two-component cationic sublayer of **TCBA** is unique in the case of halobismuthates(III). **TCBA** adopts the triclinic space group () at 100 K. Differential scanning calorimetry (DSC) and dilatometric measurements showed that it undergoes reversible first-order phase transition (PT) at 420/405 K (heating/cooling) governed by an 'order-disorder' mechanism. The crystal structure of **TBC** (*Cmca* at 100 K) contains the chains of *cis*-connected octahedra and a hydrogen-bonded array of 1,2,4-triazolium cations. The statistical disorder of the 1,2,4-triazolium cations is found at low temperatures. No PT is detected between 100 and 400 K in **TBC**.

Słowa kluczowe

A. halides, X-ray diffraction, dielectric properties

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