

Structural characterization, thermal, dielectric, vibrational properties and molecular dynamics of $(C_5H_5NH)_3BiCl_6$.

Autorzy

Jolanta Tarasiewicz

Ryszard Jakubas

Grażyna Bator

J. Zaleski

Jan Baran

Wojciech Medycki

Rok wydania

2009

Czasopismo

Journal of Molecular
Structure

Numer woluminu

932

Strony

6-15

DOI

10.1016/j.molstruc.2009.05.034

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

$(C_5H_5NH)_3BiCl_6$ crystallizes at room temperature in the triclinic space group $P\bar{1}$. The crystal is built up of the separated $BiCl_6^{3-}$ octahedral anions and pyridinium cations. Differential scanning calorimetry (DSC) and dilatometric measurements disclose structural phase transition of first-order type at 265/302 K (cooling/heating). The dielectric investigations reveal a step-wise change of the electric permittivity at T_c characteristic of the crystals with the high-temperature plastic-like phase. Temperature-dependent infrared spectra for polycrystalline samples have been taken between 20 and 306 K to clarify the cation dynamics contribution to the mechanism of the phase transition. The modes assigned to the deformation vibration of the NH^+ group in the pyridinium ring appear to be the most sensitive to the phase transition. The possible molecular motions of the $C_5H_5NH^+$ cations are studied by the proton magnetic resonance (1H NMR).

Słowa kluczowe

X-ray, Phase transition, 1H NMR, Infrared, Dielectric,
Pyridinium

Adres publiczny

<https://doi.org/10.1016/j.molstruc.2009.05.034>

Strona internetowa wydawcy

<http://www.elsevier.com>

