Internal dynamics of $(C_3N_2H_5)_5Bi_2Cl_{11}$ studied by IINS, ^1H NMR and QC methods.

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The low temperature inelastic incoherent neutron scattering spectra of pentakis (imidazolium) undecachlorodibismuthate (III) $[(C_3N_2H_5)_5Bi_2Cl_{11}]$ were discussed versus different models of reference structures obtained by quantum chemical calculations in the energy transfer range up to 1200 cm^{-1}. The second moment of ^1H NMR line and spin–lattice relaxation times were employed to study the internal dynamics of imidazolium cation at the ferroelectric–paraelectric phase transition.

Słowa kluczowe

Imidazolium undecachlorodibismuthate (III), Inelastic incoherent neutron scattering, DFT calculations, Internal dynamics by 1H NMR method

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