Structure, phase transitions and molecular dynamics in 4-methylpyridinium tetrachloroantimonate(III), [4-$CH_3C_5H_4NH$][$SbCl_4$].

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Streszczenie

Crystal structure of the 4-methylpyridinium tetrachloroantimonate(III), [4-$CH_3C_5H_4NH$][$SbCl_4$], has been determined at 240 K by X-ray diffraction as monoclinic, space group, $P2_1/n$, Z=8. Differential scanning calorimetry and dilatometric studies indicate the presence of two reversible phase transitions of first order type, at 335/339 and 233/289 K (cooling/heating) with ΔS=0.68 and 2.2 J mol^{-1} K^{-1}, respectively. Crystal dynamics is discussed on the basis of the temperature dependence of the ^1H NMR spin–lattice relaxation time T_1 and infrared spectroscopic studies. The low temperature phase transition at 233 K of an order–disorder type is interpreted in terms of a change in the motional state of the 4-methylpyridinium cations. The phase transition at 335 K, probably of a displacive type, is characterised by a complex mechanism involving the dynamics of both the cationic and anionic sublattice. The ^1H NMR studies show that the low temperature phase III is characterised only by the dynamics of the CH_3 groups.

Słowa kluczowe

D. Phase transitions, D. Nuclear magnetic resonance, D. Dielectric properties, C. Infrared spectroscopy

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