

Structure, phase transitions and molecular dynamics in 4-methylpyridinium tetrachloroantimonate(III), [4-CH₃C₅H₄NH][SbCl₄].

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Streszczenie

Crystal structure of the 4-methylpyridinium tetrachloroantimonate(III), [4-CH₃C₅H₄NH][SbCl₄], 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 $\Delta S=0.68$ and $2.2 \text{ J mol}^{-1} \text{ K}^{-1}$, 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 CH₃ groups.

Słowa kluczowe

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