Structure, phase transitions and molecular motions in 4-aminopyridinium perchlorate.

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Streszczenie

The crystal structure of the 4-aminopyridinium perchlorate (4-apyH)ClO_4 has been determined at 100 K by means of x-ray diffraction as monoclinic, with space group $P\ 2_1$, with $Z = 8$. The crystal undergoes two structural phase transitions: one of first-order type, reversible, at 241/243 K (on cooling/heating respectively) and one of weakly first-order type, irreversible, at 277 K (on heating). The crystal dynamics is discussed on the basis of the temperature dependence of the ^{1}H nuclear magnetic resonance second moment (M_2) and spin–lattice relaxation time T_1. Both phase transitions are interpreted in terms of the changes in the motional state of $(4\text{-apyH})^+$ cations and ClO_4^- anions. The dielectric dispersion studies disclose a relaxation process over the high-temperature phase (above 241 K) in the audio-frequency region. The dielectric results are described by a Cole–Cole equation. The title crystal reveals pyroelectric properties below 241 K. The ferroelastic domain structure of (4-apyH)ClO_4 is observed over the whole temperature range studied

Adres publiczny

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