Crystal structure, phase transition, and disorder in pyridinium methanesulfonate.

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Streszczenie

Thermal analysis, X-ray diffraction and vibrational spectroscopy have been used to investigate pyridinium methanesulfonate in order to verify its crystal structure and to have insight into its anomalous dynamical properties. This compound undergoes a solid-solid, reversible phase transition at 255.8/266.8 K (cooling/heating). It crystallizes in non-centrosymmetric Pna21 space group at the high-temperature phase (I) and in centrosymmetric Pbca one at the low-temperature phase (II). The entropy gain occurred at the II→I transition has shown that two independent orientations of ions in the disorder phase (I) are allowed. Infrared spectra have confirmed that the pyridinium cation as well as the –CH3 group of the anion exhibit changes in their dynamics when entering the phase I. These spectra have also suggested residual disorder of both, the pyridinium cation and the –CH3 group, in the low temperature phase (II).

Słowa kluczowe

Pyridinium, Methanesulfonate, hydrogen bonds, dSC, Temperature-dependent IR spectra, phase transition, Disorder

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