Experimental (IR) and theoretical (LDA) studies of the structure and vibrational-reorientational dynamics of ferroelastic 1-aminopyridinium iodide.

Autorzy

Magdalena T. Owczarek

Ryszard Jakubas

Irena Majerz

Jan Baran

Rok wydania

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Streszczenie

Calculations of the molecular structure and normal vibration frequencies have been performed using ADF (Amsterdam Density Functional) program package for initial structural data of 1-aminopyridinium iodide, $(1\text{-}NH_2C_5H_5N)^+I^-$, low temperature phase (110 K). Cambridge Structural Database survey has been carried out in order to explore hydrogen bond patterns of 1-aminopyridinium ring and to analyze the strength of intermolecular N–H···I^- interactions. Infrared spectra of powdered $(1\text{-}NH_2C_5H_5N)^+I^-$ in a frequency range 4000–400 cm^{-1} in a wide temperature region (from 300 to 413 K), covering ferroelastic-paraelastic phase transition at 384/383 K (heating/cooling), are presented and analyzed. The mechanism of the phase transition is discussed.

Słowa kluczowe

ADF program, N–H···I hydrogen bond, 1-Aminopyridinium, phase transition, Infrared

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