Phase transitions in non-centrosymmetric pyridinium trifluoromethanesulfonate crystal : vibrational studies.

Autorzy

Dominik M. Jesariew

Maria M. Ilczyszyn

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Streszczenie

Infrared spectroscopy (4000–400 cm^{-1}) in the wide temperature range, from 11 to 473 K, has been used to investigate the non-centrosymmetric pyridinium trifluoromethanesulfonate crystal, exhibiting several phase transitions. The assignments of the bands observed in the studied spectra have been proposed. The temperature dependence of the wavenumbers and the full width at half maximum (FWHM) of the bands arising from some internal vibrations of the pyridinium cation and the triflate anion have been analyzed in order to achieve a knowledge of whether these both ions are involved in the phase transitions and what is the role of these both ions in these phase transitions. The infrared measurements showed that the both ions, pyridinium cation and triflate anion are involved in the high temperature phase transitions of the order–disorder type, previously reported at 305.1 and 396.7 K. They also revealed that these transitions are governed by a rotational mobility (changes in dynamical states) of both the pyridinium and triflate ions. Our results show that the multiple structures of the νNH and νND bands observed in the studied infrared spectra is due to the Fermi resonance interaction between the stretching vibration of the N–H···O hydrogen bond and the overtones and combinations of the internal vibrations of the pyridinium cation.

Słowa kluczowe

Pyridinium trifluoromethanesulfonate, vibrational spectroscopy, Temperature-dependent infrared spectra, Order–disorder phase transition, Ion mobility

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