The crystal structure and the phase transitions of pyridinium trifluoromethanesulfonate.

Autorzy

Dominik M. Jesariew

Maria M. Ilczyszyn

Adam Pietraszko

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Streszczenie

The calorimetric and optical studies and the structural properties of pyridinium trifluoromethanesulfonate (abbreviated as PyHOTf) are reported. A sequence of four fully reversible solid–solid phase transitions, at 223.0, 309.0, 359.9 and 394.3 K, has been discovered. The phase transition sequence was confirmed by x-ray diffraction data. The crystal structures of three phases (V, IV and III) have been determined from the single crystal x-ray diffraction data. Structural properties of the high temperature phases are characterized using powder x-ray diffraction data measured in the 290–425 K temperature range. The structural changes triggered by the temperature change are discussed in relation to the phase transitions. Two low temperature phases (V and IV) belong to the P43212 space group of the tetragonal system. The intermediate phases (III and II) are monoclinic and the prototype high temperature phase (I) is a pseudo-cubic (tetragonal) one. The low temperature phases (V and IV) are well ordered. The crystal structure of intermediate (III and II) and prototype (I) phases are characterized by high disorder of the pyridinium cations and triflate anions.

Adres publiczny

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