Order-disorder phase transitions and their influence on the structure and vibrational properties of new hybrid material: 2-amino-4-methyl-3-nitropyridinium trifluoroacetate.

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Streszczenie

New organic–organic salt, 2-amino-4-methyl-3-nitropyridinium trifluoroacetate, has been synthesised and characterised by FT-IR, FT-Raman, DSC and single crystal X-ray crystallography. The 2-amino-4-methyl-3-nitropyridinium trifluoroacetate undergoes a reversible phase transition at ∼162 K. The X-ray structures, vibrational spectra and quantum chemical DFT calculations (B3LYP/6-31G(d,p) approach) have been analysed for high-temperature and low-temperature modifications of the compound, which both crystallize in orthorhombic space group Pbca with two non-equivalent cations and two anions in the asymmetric unit. Their crystal and molecular structures have been compared and the role of the intermolecular interactions in these crystals has been analysed. The mechanisms of the phase transition have been proposed.

Słowa kluczowe

2-Amino-4-methyl-3-nitropyridinium trifluoroacetate, Hybrid organic salt, XRD studies, TD DFT calculations, Vibrational spectra, phase transitions

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