Comprehensive physicochemical studies of a new hybrid material: 2-amino-4-methyl-3-nitropyridinium hydrogen oxalate.

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Kolekcja

Naukowa

Streszczenie

A new organic–organic salt, 2-amino-4-methyl-3-nitropyridinium hydrogen oxalate (**AMNPO**), and its deuterium analogue have been synthesized and characterized by means of FT-IR, FT-Raman, DSC and single crystal X-ray studies. The DSC measurements and temperature dependence of the IR and Raman spectra in the range 4–295 K show that it undergoes a reversible phase transition at ~240 K. At room temperature it crystallizes in noncentrosymmetric space group $P2_1$. The unit-cell is built of the 2-amino-4-methyl-3-nitropyridinium cations and oxalate monoanions which are connected *via* the NH···O and OH···O hydrogen bonds. The geometrical and hydrogen bond parameters are similar for non-deuterated (at 120 and 293 K) and deuterated compounds (at 90 K). The phase transition is probably a consequence of order–disorder transition inside of hydrogen network. The 6-311G(2d,2p) basis set with B3LYP functional have been used to discuss the structure and vibrational spectra of the studied compound.

Słowa kluczowe

2-Amino-4-methyl-3-nitropyridinium hydrogen oxalate, Deuterated salt, Temperature dependence, IR and Raman spectra, Crystal structure

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