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The role of hydrogen bonds in the crystals of 2-amino-4-methyl-5-nitropyridinium trifluoroacetate monohydrate and 4-hydroxybenzenesulfonate – X-ray and spectroscopic studies.

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Two new organic–organic salts, 2-amino-4-methyl-5-nitropyridinium trifluoroacetate monohydrate (AMNP-TFA), and 2-amino-4-methyl-5-nitropyridinium 4-hydroxybenzenesulfonate (AMNP-HBS), were obtained and characterized by means of FT-IR, FT-Raman and single crystal X-ray crystallography. In the former crystal, the cations, anions and water molecules are linked into layers by three types of hydrogen bonds, $N_PH\cdots O$, $N_AH\cdots O$ and $OH\cdots O$. These layers are connected by weaker $CH\cdots O$ hydrogen bonds. In the latter crystal, the cations and anions form one-dimensional structure through a number of hydrogen-bonding interactions involving the OH, NH^+ and NH_2 groups as donors. In this case the $N_PH\cdots O$ and $N_AH\cdots O$ hydrogen bonds are formed. The combination of interactions between cations and anions results in the formation of columns. Additionally, there are π–π stacking interactions between the columns. The obtained X-ray structural data are related to the vibrational spectra of the studied crystals.

Słowa kluczowe

2-Amino-4-methyl-5-nitropyridinium trifluoroacetate monohydrate, 2-Amino-4-methyl-5-nitropyridinium 4-hydroxybenzenesulfonate, Hydrogen bonds, IR and Raman spectra, X-ray study, Quantum chemical calculations

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