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Extremely different structures and vibrational spectra of tetramethylpyrazine nitrate dihydrate in solid and solutions.

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Streszczenie

The subject of the study is the crystal structure of 2,3,5,6-tetramethylpyrazine (TMP) nitrate dihydrate in which two types of hydrogen bonds are formed, namely $^{+}$N–H···O between protonated tetramethylpyrazine and water as well as between OH group (in water molecule) and oxygen atom of the nitrate anion. The structure is well reflected both in infrared and Raman spectra. Particularly clear picture of broad bands above 2000 cm^{-1} is visible. The experimental and calculated Raman spectra are in a relatively good agreement. This crystal structure changes dramatically if the hydrogen-bonded complex is dissolved. In acetonitrile it dissociates with formation of the intermolecular $(N–H···N)^{+}$ hydrogen bonds between two TMP molecules, and free water molecules. In methylenchloride, besides the intermolecular $(N–H···N)^{+}$ hydrogen bonds, the formation of $(O···H···O)^{+}$ species between two water molecules is established.

Słowa kluczowe

tetramethylpyrazine nitrate dihydrate, X-ray structure, FT-IR spectroscopy, Raman spectroscopy, DFT calculation

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