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The dehydration process in the DL-phenylglycinium trifluoromethanesulfonate monohydrate crystal revealed by XRD, vibrational and DSC studies.

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Streszczenie

Thermal analysis, X-ray diffraction and temperature-dependent IR spectroscopy were used to study the dehydration process of crystalline DL -phenylglycinium trifluoromethanesulfonate monohydrate (PGTFH), C8H10NO2+·CF3SO3−·H2O. PGTFH dehydrates in one step centred at 353 K and crystallizes in the monoclinic space group C2/c, whereas the anhydrous compound (PGTF) crystallizes in the triclinic space group P[\overline{1}]. The dehydration process in PGTFH is preceded by a weakening of both the noncovalent aromatic–aromatic interactions and the packing contacts. This process is accompanied by the breakage of medium-strength O—H···O hydrogen bonds between ions inside layers and a reorganization of the ions within the layers. This reorganization results in the formation of two different ion pairs (DL -phenylglycinium trifluoromethanesulfonate) and the formation of a new hydrogen-bond network. The dehydration process does not destroy the nature of the crystal structure. Both crystals, i.e. hydrated and anhydrous, have a layered structure, although the layers of each crystal are arranged somewhat differently.

Słowa kluczowe

phenylglycinium, trifluoromethanesulfonate, dehydration, crystal structure

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