X-ray diffraction, spectroscopic (IR, Raman) and DSC studies of bis (betainium) *p*-toluenesulfonate monohydrate crystal.

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Streszczenie

Bis(betainium) *p*-toluenesulfonate monohydrate (abbreviated as BBTSH) was studied at various temperatures by X-ray diffraction, differential scanning calorimetry and vibrational spectroscopy methods. DSC curves of BBTSH show a peak at about 349 K which corresponds to water escape from the crystal, and reveal the “cold crystallization” phenomenon. BBTSH crystallizes in the $P2_1/c$ space group of monoclinic system. After heating above 349 K the compound dehydrates, the crystal system changes to triclinic, the monocrystalline samples become non-merohedral twins. The BBTSH crystal comprises *p*-toluenesulfonic anions, monoprotonated betaine dimers and water molecules. Three kinds of hydrogen bonds are present in the crystal: strong, asymmetric and almost linear OH···O hydrogen bond (R(O···O) = 2.463(2) Å), weak $O_wH\cdots O$ hydrogen bonds (R(O_w···O) = 2.820(2) − 2.822(2) Å) and weak CH···O hydrogen bonds (R(C···O) = 3.295(2) − 3.416(2) Å). The ν_aOHO vibration of the strongest hydrogen bond in the crystal gives rise to an intense broad absorption with numbers of transmission windows in the low wavenumber region of the infrared spectra. Coupling between νCO stretching vibrations of two COO groups of the betaine dimer was detected. The process corresponding to the loss of water is accompanied by the breakage of strong OH···O hydrogen bonds in betaine dimers and rearrangement inside half of the betaine dimers. This rearrangement results in formation of the new betaine dimers with OH···O hydrogen bond of similar strength as corresponding bond in the hydrated form (BBTSH).

Słowa kluczowe

hydrogen bonds, infrared spectra, single crystal Raman spectra, Betaine dimer, Twinned structure, dehydration process