Glycine-methanesulfonic acid (1:1) and glycine-*p*-toluenesulfonic acid (1:1) crystals: comparison of structures, hydrogen bonds, and vibrations.

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Streszczenie

The crystal structures of glycine–methanesulfonic acid (1:1) and glycine–*p*-toluenesulfonic acid (1:1) have been investigated by X-ray diffraction at 293 K. They belong to centrosymmetric: (i) $P2_1/n$ space group of monoclinic system and (ii) *Pbca* space group of orthorhombic system, respectively. Both crystals consist of glycinium–sulfonate dimers (methane- or *p*-toluenesulfonate, respectively) with medium-strong and very similar O–H···O hydrogen bonds. N–H···O bonds connect glycinium–sulfonate dimers into infinite chains. Both sulfonic acids reveal very similar acidic properties. In glycine–*p*-toluenesulfonic acid (1:1) crystal very weak, C–H···π improper hydrogen bonds are formed. Vibrational spectra of the crystals are related to their structures.

Słowa kluczowe

Glycine–methanesulfonic acid crystal, Glycine–p-toluenesulfonic acid crystal, Vibrational spectra, X-ray diffraction, DSC, Hydrogen bond, Improper hydrogen bond, Blue shift, Acidity

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