



β -alanine-hydrochloride (2:1) crystal: structure,¹³ C NMR and vibrational properties, protonation character.

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The crystal structure of β -alanine–hydrochloride (2:1) complex (2A-HCl) has been determined by X-ray diffraction method at 298 and 100 K as monoclinic, space group $C2/c$, $Z=4$. The crystal comprises chloride anions and protonated β -alanine dimers: two β -alanine zwitterions are joined by strong, symmetric (C_i) hydrogen bond with the $O\cdots O$ distance of 2.473 Å at room temperature. Powder FT-IR and FT-Raman as well as solid state ¹³C NMR spectra provide insights into the solid structure of this complex, character of its hydrogen bonds and the β -alanine protonation.

Adres publiczny

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