

Vibrational, XRD and ^{13}C NMR studies of DL-phenylglycinium methanesulfonate crystal.

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Streszczenie

A new crystal formed by DL-phenylglycine and methanesulfonic acid (PGLYMS) was obtained and studied by X-ray diffraction, IR and Raman spectroscopy, solid state NMR and DSC methods. Additionally, theoretical computations for the phenylglycine cation were carried out (DFT/B3LYP/aug-cc-pVDZ). Our results show that PGLYMS does not exhibit any phase transitions and crystallizes in the $P2_1/c$ space group of monoclinic system ($Z=4$). Detailed analysis of its structure and its IR, Raman and NMR spectra is presented

Słowa kluczowe

hydrogen bonds, IR spectroscopy, Methanesulfonic anion, Phenylglycinium cation, Solid state NMR spectroscopy

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