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Vibrational, structural and theoretical studies of potassium DL-phenylglycinate.

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Streszczenie

Phenylglycine, the simplest aromatic amino acid is interesting because of its potential applications as medical agent involved in the alkali ions transport in the biological and medical systems. Rather scarce structural and spectroscopic data concerning this molecule encouraged us to study a crystal structure and vibrational properties of the potassium dl-phenylglycinate salt (PGLYK). The crystal structure of PGLYK has been determined by X-ray diffraction at 100 K as monoclinic, space group $P2_1/c$, with $Z = 4$. The crystal comprises phenylglycine anions (PGLYA) and potassium cations. Each K^+ is surrounded by five oxygens and one nitrogen which form a distorted octahedron. The intramolecular N–H⋯O hydrogen bond of 2.713(2) Å length is present in the studied crystal. The intermolecular N–H⋯π contacts have also been detected between adjacent amino groups and phenyl rings which may have an important contribution to the molecular packing observed for PGLYK. The infrared and Raman spectra of the crystalline sample are presented and discussed in relation to the theoretical predictions performed for the phenylglycine anion and potassium phenylglycinate at the B3LYP/6-311++G(2d,2p) level. The detailed interpretation of the vibrational spectra has been made on the basis of the calculated potential energy distribution matrix (PED).

Słowa kluczowe

Molecular structure, Vibrational spectra, DFT calculation, Potassium dl-phenylglycinate

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