Synthesis, crystal structures and spectral characterization of imidazo [1,2-*a*]pyrimidin-2-yl-acetic acid and related analog with imidazo[2,1-*b*]thiazole ring.

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Streszczenie

Imidazo[1,2-*a*]pyrimidin-2-yl-acetic acid (H*IPM-2-ac*) and its analog with imidazo[2,1-*b*]thiazole ring (H*ITZ-6-ac*) were synthesized and structurally characterized by single-crystal X-ray diffraction corroborated with calculations of Hirshfeld surfaces, which provided detailed insight into intermolecular interactions constituting both crystals. The IR and Raman spectra of H*IPM-2-ac* and H*ITZ-6-ac* were recorded and interpreted in details with the aid of Density Functional Theory (DFT) calculations and Potential Energy Distribution (PED) analysis of computed normal vibrations. Special attention was paid on hydroxyl and methylene groups involved in hydrogen bonds, which vibrations were monitored by H/D substitution. Recrystallization of parent compounds from deuterium oxide (D_2O) solutions resulted in deuteration of their carboxylic OH groups and almost complete deuteration of H*IPM-2-ac* methylene group. The latter phenomenon is clearly reflected in the vibrational spectra and confirmed by ^1H NMR experiments in solution.

Słowa kluczowe

imidazo[1,2-a]pyrimidine, Single-crystal X-ray diffraction, hirshfeld surface analysis, density functional calculations, vibrational spectroscopy

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