Derivatives of benzo[*b*]furan. Part II. Structural studies of derivatives of 2- and 3-benzo[*b*]furancarboxylic acids.

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Streszczenie

The selected derivatives of the 2- and 3-benzo[*b*]furancarboxylic acids were synthesized and their structures were studied using the X-ray crystallography and the computational methods. The monocarboxylic acids (**1**–**3**) crystallize as dimers stabilized by the O–H···O intermolecular hydrogen bonds. Moreover, intramolecular hydrogen bonds are formed between the OH and C(=O)CH_3 groups, substituted to the aromatic ring (**2**–**4**). In the crystal structures of**1**–**4**, weak C–H···O, C–H···π, and C–H···Br interactions stabilize the three-dimensional packing of molecules. The crystalline sodium complex of **1** has the stoichiometry [**Na** $^+$ ·**1A** $^-$ ·**1B**]·**1C**, thus, the asymmetric unit contains three different moieties of **1**. In this complex, the Na^+ cation is hexacoordinated having a strongly distorted tetragonal bipyramidal polyhedron. For each molecule **1**–**4**, several conformers were obtained in the gas phase. It was achieved by the rotations of substituents [COOR and/or C(=O)CH_3, where R = H, CH_3] with respect to the rigid benzo[*b*]furan system. As indicated by the quantum-chemical calculations, the solid-state conformers for **3** and **4** (3-benzo[*b*]furancarboxylic acid derivatives) are the most stable ones. In contrast, the solid-state conformers of the 2-benzo[*b*]furancarboxylic acid derivatives (**1**, **2**) have the energies higher than the lowest energy conformer by 1.23 and 0.69 kcal/mol, respectively. It seems that intermolecular contacts in the crystal influence on the orientation of substituents, and the conformers observed in the sodium complex of **1** provide evidence of such flexibility.

Słowa kluczowe

Benzo(b)furan derivatives, conformational analysis, theoretical calculations, crystal structure