



Very Strong Hydrogen Bond in Nitrophthalic Cocrystals

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Streszczenie

This work presents the studies of a very strong hydrogen bond (VSHB) in biologically active phthalic acids. Research on VSHB comes topical due to its participation in many biological processes. The studies cover the modelling of intermolecular interactions and phthalic acids with 2,4,6-collidine and N,N-dimethyl-4-pyridinamine complexes with aim to obtain a VSHB. The four synthesized complexes were studied by experimental X-ray, IR, and Raman methods, as well as theoretical Car–Parrinello Molecular Dynamics (CP-MD) and Density Functional Theory (DFT) simulations. By variation of the steric repulsion and basicity of the complex' components, a very short intramolecular hydrogen bond was achieved. The potential energy curves calculated by the DFT method were characterized by a low barrier (0.7 and 0.9 kcal/mol) on proton transfer in the OHN intermolecular hydrogen bond for 3-nitrophthalic acid with either 2,4,6-collidine or N,N-dimethyl-4-pyridinamine cocrystals. Moreover, the CP-MD simulations exposed very strong bridging proton dynamics in the intermolecular hydrogen bonds. The accomplished crystallographic and spectroscopic studies indicate that the OHO intramolecular hydrogen bond in 4-nitrophthalic cocrystals is VSHB. The influence of a strong steric effect on the geometry of the studied cocrystals and the stretching vibration bands of the carboxyl and carboxylate groups was elaborated.

Słowa kluczowe

very strong hydrogen bond, phthalic acid, steric effect, CP-MD, DFT

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