

Impact of intermolecular hydrogen bond on structural properties of phenylboronic acid: quantum chemical and X-ray study.

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Streszczenie

The molecular structure and properties of phenylboronic acid were investigated experimentally using X-ray structural analysis and spectroscopic methods. Infrared (IR) spectroscopy measurements were performed to assess the hydrogen bonding strength. The experimental part is enhanced by computational results concerning the geometrical and electronic structure. The molecular dimer (basic structural motif) was investigated on the basis of density functional theory (DFT) and Møller-Plesset second order (MP2) perturbation theory. The basis-set superposition error (BSSE) was calculated to correct the binding energy. Atoms in molecules (AIM) and topological analysis of electron localization function (ELF) were applied to study the intermolecular hydrogen bond properties and localization pattern for the neighborhood of the boron atom. The anharmonicity of the hydrogen bond potential function was studied by solving the time-independent Schrödinger equation. Potential energy distribution (PED) analysis of the normal modes was performed to identify the characteristic frequencies of the studied system. Subsequently, the interaction energy for the dimeric form was decomposed using the symmetry-adapted perturbation theory (SAPT) scheme. Car-Parrinello molecular dynamics (CPMD) gave an insight into dynamical processes occurring in the phenylboronic acid dimer in vacuo. The hydrogen bridge protons in the phenylboronic acid are not shifted significantly toward the acceptor. Lower dimerization energy with respect to the carboxylic acid dimers is explained on the basis of the interaction energy decomposition as the effect of diminished induction term. The employment of SAPT and CPMD approaches is a step forward in the understanding of the physico-chemical nature of the large family represented by the investigated compound.

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