The nature of hydrogen bonding in selected hydrazide derivatives investigated *via* static models and Car-Parrinello molecular dynamics.

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The geometric and spectrocopic properties of 2-hydroxy-thiobenzhydrazide and 2-hydroxy-benzhydrazide were investigated within the frame work of Density Functional Theory (DFT). Special attention was devoted to the description and analysis of intra- and intermolecular hydrogen bonds. The choice of the compounds was dictated by their structural similarity and the presence of two types of hydrogen bridges: O–H...S (in 2-hydroxy-thiobenzhydrazide, less common) and O–H...O (in 2-hydroxy-benzhydrazide). The latter could be classified as a low-barrier hydrogen bond (LBHB). First the DFT method was used to obtain the geometric parameters for the monomeric and dimeric forms of the compounds at various levels of theory. Then the binding energy was calculated for the dimeric forms to estimate the strength of the intermolecular hydrogen bonds. Atoms in Molecules (AIM) theory was applied to show quantitatively how the formation of the intermolecular hydrogen bonds affects the strength of the intramolecular hydrogen bonds. The electron density and its Laplacian were calculated for the bond critical points defining the H-bridges. Car-Parrinello molecular dynamics (CPMD) was then used to investigate the changes in the geometric parameters as a function of simulation time. This part of the computational study was performed in vacuo and in the solid state. The vibrational properties of the investigated hydrazides were obtained via Fourier transform of the autocorrelation functions of the dipole moment and atomic velocity. It was found that the formation of the intermolecular H-bonds does not significantly affect the strength of the intramolecular H-bonds. There fore inductive and steric effects out side the immediate vicinity of the intramolecular bridge have minor influence on its investigated properties. The application of CPMD gave a more detailed picture of the bridged protons' dynamics. The computational results agree with available experimental data. The influence of the intermolecular hydrogen bonding net work and non-bonded crystal field interactions on the vibrational features of the investigated molecules is demonstrated and discussed.

Słowa kluczowe

Hydrogen bond, BSSE, AIM, CPMD, Gas phase, solid state