

"Zwitterionic proton sponge" hydrogen bonding investigations on the basis of Car-Parrinello molecular dynamics.

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Streszczenie

1,8-Bis(dimethylamino)-4,5-dihydroxynaphthalene has been investigated on the basis of static DFT computations and Car-Parrinello molecular dynamics. The simulations were performed in the gas phase and in the solid state. The studied "zwitterionic proton sponge" possesses two, short intramolecular hydrogen bonds (O-H...O and N-H...N) classified as Low Barrier Hydrogen Bonds (LBHBs); therefore, the system studied is strongly anharmonic. In addition, the compound exists as a "zwitterion" in solution and in the solid state, thus the intramolecular hydrogen bonds belong to the class of charge-assisted interactions. The applied quantum-chemical methods enabled investigations of metric and spectroscopic parameters of the molecule. The time-evolution investigations of the H-bonding showed a strong delocalization of the bridge protons and their high mobility, reflected in the low barriers on the free energy surfaces. Frequent proton transfer phenomena were noticed. The power spectra of atomic velocity were computed to analyze the vibrational features associated with O-H and N-H stretching. A broad absorption was indicated for both hydrogen bridges. For the first time, Car-Parrinello molecular dynamics results are reported for the compound, and they indicate a broad, shallow but not barrierless, potential well for each of the bridge protons.

Adres publiczny

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<https://www.acs.org/content/acs/en.html>