On the nature of inter- and intramolecular interactions involving benzo[h]quinoline and 10-hydroxybenzo[h]quinoline: electronic ground state vs excited state study.

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Streszczenie

The inter- and intramolecular interactions of benzo[h]quinoline and 10-hydroxybenzo[h]quinoline have been studied using quantum-chemical methods. Here, we report on results of monomeric and dimeric forms obtained on the basis of Density Functional Theory (DFT) in its classical formulation as well as using its Time-Dependent extension (TD-DFT). The simulations were performed in the gas phase and with solvent reaction field using toluene and acetonitrile as solvents. Symmetry-Adapted Perturbation Theory (SAPT) and Atoms in Molecules (AIM) were employed to characterize interactions and forces present in the studied compounds with special attention paid to the presence of inter- and intramolecular hydrogen bonds. It was found that spontaneous proton transfer phenomenon was not preferable in the electronic ground state. However it was noticed in the excited electronic state. The presence of the polar environment lowers the energy profile of the proton reaction path and slightly influences the electronic structure and aromaticity of the compounds. The results of the SAPT analysis showed that the O-H... N intermolecular hydrogen bond in the dimer 1 is only ca. twice stronger than the C-H... O and C-H... π contact present in the dimers formed by 10-hydroxybenzo[h]quinoline.

Słowa kluczowe

Benzo[h]quinolone, Hydrogen bond, DFT, HOMA, SAPT, AIM, TD-DFT

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