Właściwości wewnątrzcząsteczkowych wiązań wodorowych w wybranych *N*-tlenkach pochodnych chinoliny = Intramolecular hydrogen bonds properties in selected N-oxides of quinoline derivatives.

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In the current article we would like to summarize our research shedding light onto properties of intramolecular hydrogen bonds present in N-oxide quinoline derivatives. The compounds for the current study were chosen to contain diverse types of hydrogen bonds. Therefore, in the current study we analyze three kinds of hydrogen bonding and their properties. It is well known, that the presence of intramolecular hydrogen bonds stabilizes conformations of molecules. Substituent effects (inductive and steric) influence the strength of the H-bonding as well as its features. Moreover, the intramolecular hydrogen bond in the studied N-oxides belongs to the family of resonance assisted hydrogen bonds (RAHB). Our short overview presents the summary of results obtained for twelve N-oxides of quinoline derivatives. Quantum-chemical simulations were performed on the basis of static models (classical DFT and MP2 approaches) as well as ab initio molecular dynamics (Car-Parrinello MD). The metadynamics method was applied to reproduce the maps of free energy for the motion of the bridged proton. The computations were performed in the gas and in the crystalline phases. Electronic ground state is a natural framework in which chemical compounds exist most of the time. However, in many chemical species we observe a spontaneous internal reorganization of their chemical bonds and atoms e.g. proton transfer phenomenon and the appearance of tautomeric forms already in the ground state. Therefore, it was interesting to investigate some N-oxides in the excited electron state knowing that they exhibit excited- state-induced proton transfer (ESIPT effect). At the end of the article we draw some conclusions related to the intramolecular H-bond properties present in the discussed N-oxides of quinoline derivatives.

Słowa kluczowe

DFT, density functional theory, MP2, Møller-Plesset second order perturbation method, CPMD, Car-Parrinello molecular dynamics, intramolecular HB, N-oxides of quinoline derivatives

DFT, teoria funkcjonału gęstości, MP2, metoda rachunku zaburzeń drugiego rzędu Møllera-Plesseta, CPMD, dynamika molekularna Cara-Parrinello, wewnątrzcząsteczkowe wiązanie wodorowe, N-tlenki pochodnych chinoliny