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Probing of Fluorine Atom Electronic Shell by means of Topological Analysis of Helium Chemical Shift Surfaces

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Non-covalent interactions play crucial role in structure stabilization of molecules. The ability of a molecule to partcipate in non-covalent interactions is determined by the features of its electron shell. In recent years in study of non-covalent interactions (in particular hydrogen bonds) there have been a numerous attempts to find a parameter that could describe the features of the electron shell of isolated molecule and predict some characteristics of intermolecular interactions, such as the geometry and binding energy. Such parameters as calculated quantum mechanical functions of the molecular electrostatic potential [1], electron localization [2, 3], and electron density were proposed to use the. However, the problem of finding principally measurable parameter which will be capable to describe features of the electronic shells remains an issue. In this work we propose to use ^{3}He atom as a probe particle. Our approach is to place the ^{3}He atom sequentially in a set of points around investigated molecule and calculate interaction energy and NMR parameters such as chemical shift of the helium atom δ_{He}. It is shown that the chemical shift δ_{He} is sensitive even to weak changes in the electronic shell. At first step, we calculate the surfaces of chemical shift of the helium atom δ_{He}. Further, a topological analysis of this surface is carried out. Interestingly, features of δ_{He} surface turned out to be more informative markers for hydrogen bond properties than other electronic structure parameters. As a model molecule for this work we used such simple fluorine containing proton donors FH, $(HFH)^+$ and acceptors F^-, $(FHF)^-$.

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