Nanoscale physics

Determination of the protonation center of the spiropyran molecule

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Nowadays there is fast growing interest to nano and molecular electronics. It is caused by the fact that active electronic components based on nano structures or even single molecules are very promising technological concepts. Spyropiran is a great example of such a molecule. Given its photochromic properties it can be used in devices for optical switching and storage, sensors, cell imaging etc [1].

There is a challenging problem in using spyropiran. It should be stable enough to give us full control over it. To achieve the stability of the spiropyran molecule the protonation is used.

The aim of this work is to determine the protonation center of the spiropyran and merocyanine molecules using quantum chemical calculations of electronic and energy parameters. To achieve this goal, the effective charges and electron densities on the heteroatoms have been analyzed. These values characterize an electronic structure of the molecules.

Comparing the values of the electron density at the heteroatoms can be seen that in the spiropyran molecule the difference in electron density in the atom Ospiro and N is small, and this difference is more significant in the merocyanine molecule.

The charge characteristics of the molecules show that in the merocyanine molecule the largest net negative charge concentrates on the Ospiro atom, while in spiropyran molecule Ospiro atom and N atom have almost identical negative charges.

As a conclusion we may say that in the spiropyran molecule the protonation on the Ospiro and N atoms are equiprobable. But for the merocyanine molecule O is the most possible protonation center.

1. *Singh R., Bohm M., Balasubramanian G.* Energetic and structural properties of different conformations of merocyanine and its protonated forms // Chem. Phys. Let.-2015.**-633.-**P. 287-291.