**Kovalenko O.A.,**
**Lopatkin Yu.M.,**
*Department of General and Theoretical Physics, Sumy State University, Rymsky-Korsakov St., 2, Sumy 40007, Ukraine*
**Kondratenko P.O.**
*Department of Theoretical Physics, Aerospace Institute, National Aviation University, Kosmonavt Komarov Prosp., 1, Kiev 03680, Ukraine*

# COMPUTATIONAL STUDY OF THE REACTIVITY OF THE SPIROPYRAN MOLECULE

To date, a central position in nanotechnologies takes up a design of molecular electronic devices such as switches, rectifiers, molecular wires, etc. The important components of these devices are photochromic materials due to their nanoscale dimensions. One of such materials is spiropyran molecule (SP). The SP molecule can transform to the merocyanine molecule without irradiation influence. This is possible by protonation of the SP molecule in weak acids. However, it remains unclear what is the protonation center of the SP molecule.

The aim of this work is the investigation of the electrophilic center of the SP molecule.

Proton acts as electrophile. Thus, it attacks for the place with greater electron density in the nucleophile molecule. As it is known, heteroatoms are the potential protonation centers. Hence, in the SP molecule we should consider 5 atoms as a possible center for protonation: N (11), O(30), N (37), O (41), O (42).

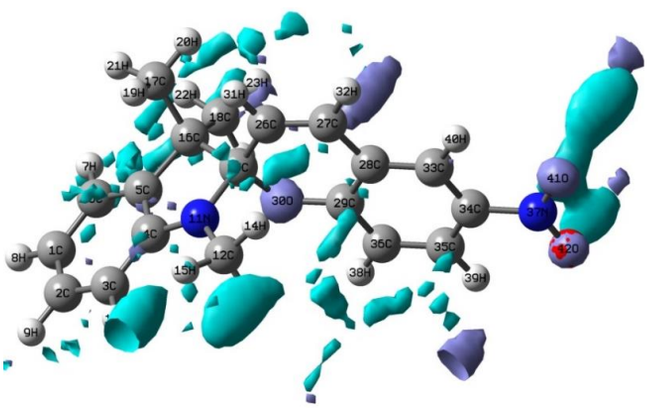


*Figure. Density difference map of the SP.*

For this reason the density difference map has been calculated on CAMB3LYP/6-31g(d) level. From Figure it can be seen that the greatest density concentrates on the O (30) and O (41). As a conclusion we may say that the most preferable center for the protonation in the SP molecule will be O (30). If proton joins to another heteroatom as N (11) it will immediately go to the O (30). If it joins to N (37) it will go to O (41).