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Proton Transfer Route in Spiropyran Molecule

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At present researches of photosensitive molecules become more popular. Such molecules are used as molecular switches, thermal and chemical sensors, etc.

One of the brightest representatives of such molecules are spiropyrans. To identify the mechanism of photochromism processes of isomerization of the spiropyran molecules have been widely studied, but the influence of protonation on this process has been studied insufficiently.

In this work we considered protonation of the spiropyran molecule at the N and O atoms and calculated the potential surface of the proton transfer route from the nitrogen atom to the oxygen atom using semiempirical method AM1 of program package MOPAC2012.

Fig.1 shows that, joining of a proton to N and O is almost equally probable. In a case when the proton is at nitrogen atom, the only obstacle to the merocyanine form is the barrier for proton transfer from N to O, which is about 2,5 eV.

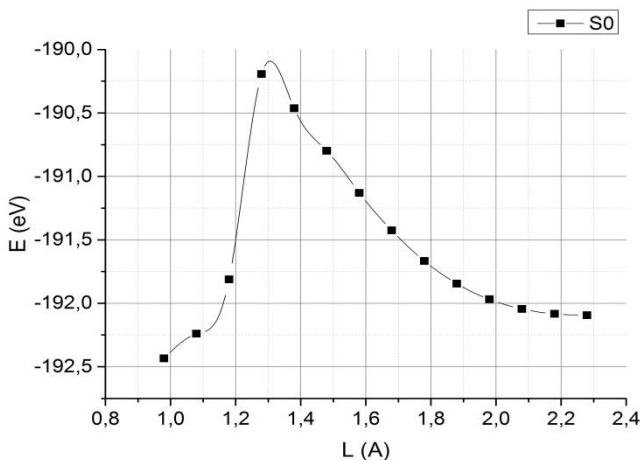


Figure 1 –
The dependence
of the energy on
the reaction
coordinate
at the proton
transfer with
forming the final
products of
reaction.

The cause of the barrier is discussed.