An ab initio MO-MD Study on Photoinduced Cis-Trans Isomerization and Intramolecular Hydrogen Atom Transfer of 2'-Hydroxychalcone

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The reaction mechanism of the one-way isomerization of 2'-hydroxychalcone was studied by calculating the potential energy surfaces of the twist of C=C double bond and the intramolecular hydrogen atom transfer in the excited triplet state by UB3LYP/6-31G** level.

The overview of the potential surface along the torsion angle and O-H bond length is depicted in Figure 1. The potential energy curve of the triplet state between the normal forms (trans-2HC and cis-2HC) exhibits the mutual isomerization. The potential energy curve between the tautomers (trans-2HC' and cis-2HC') show the one-way isomerization from cis to trans isomers. The hydrogen atom transfer had small energy barriers (< 2 kcal mol-1) in both trans- and cis-2HC. Electronic spins localize around the C=C double bond in the intermediate states (p-2HC and p-2HC') of isomerization. During the hydrogen atom transfer, electronic spins shift from the phenyl group to the 2-hydroxyphenyl moiety. The electronic charge on hydrogen bonded proton did not change significantly during the hydrogen atom transfer process.



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