

Excited-State Intramolecular Proton Transfer in triphenylimidazolic compounds

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Abstract: The excited state intramolecular proton transfer (ESIPT) of compounds derived from triphenylimidazole was investigated based on the density functional theory (DFT). Structural parameters, as bonds and angles in the fundamental and excited states, potential energy surfaces for the proton transfer, as well as, IR and UV-vis spectra and correlated electronic properties have been obtained. For compounds with electron donor substituents character, the intramolecular hydrogen bond is strengthened in the excited state and the opposite effect is observed for compounds that have electron withdrawing substituents. This observation is confirmed by -OH stretching bands in vibrational spectra. From the analysis of the electronic spectra it can be seen that the effects of the substituents clearly affect the electronic density of the compounds in the excited state S₁. The analysis of the atomic charges was fundamental to understand how the proton transfer process occurs in the excited state: in the ground state, the oxygen atom is more negative than the imidazole nitrogen atom, while, in the excited state S₁, the oxygen atom becomes less negative and the nitrogen atom becomes more negative, which favors the proton transfer. The potential energy surfaces for the proton transfer were calculated for the fundamental and excited states. There is no energy barrier in the excited state for some compounds, and a very low barrier for others. However, for the compounds with withdrawing substituents, the barriers to the proton transfer become larger.

Key-words: proton transfer, excited state, DFT, triphenylimidazole.

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