

## **DFT Studies on the Mechanism of the Michael Reaction: thiolates with acrylonitrile like acceptor.**

Kemel Arafet Cruz\*, América García López\*, Ramón Carrasco Velar\*\*.

\*Department of Chemistry, Natural Sciences Faculty, Oriente University,  
Santiago de Cuba, Cuba, CP 90500, Cuba, arafet@cnt.uo.edu.cu

\*\* Informatics Sciences University  
Havana, Cuba

### **Abstract**

The Potential Energy Surface (PES) of the addition of thiolates and aminothiolates anions to acrylonitrile like Michael acceptor at the B3LYP/6-31G(d,p) theory level is studied, the feasibility of the reaction is analyzed through the NBO charge densities, the chemical potential and the hardness calculated starting from the energy of the HOMO and LUMO orbitals; it is evaluated the reactivity of different nucleophiles and Michael acceptors using these reactivity parameters. The PES is characterized firstly by the formation of a prereactive complex (PC), this is formed for the stabilization in a minimum energy local of the reactants; this molecular association is determined by the formation of two hydrogen bonds (HB), the system evolves for a transition state (TS) until the formation of the tetrahedral intermediary (TI) charged negatively in the carbon 2, the determined activation energy is low and very similar. The analysis NBO sample in a general way for all the nucleophiles high charge densities on the electronegative atoms of S and O that they favour the interaction with the acrylonitrile H atoms, which are faulty of electrons the electroattractor effect of the  $-\text{CN}$  group. The great difference between the values of potential of the nucleophiles and studied electrophiles and the small difference in the hardness shows that in a general way the transfer of electrons is favoured from the nucleophiles to the electrophiles, and the thiolate anions they present bigger nucleophilic power than the aminothiolate anions.