Abstract

We have investigated the hydrogen isotope effect on the geometry, the electronic structure and the stability of the borane-carbonile adduct, by using the nuclear-electronic molecular orbital method (NEMO) which has been implemented in the APMO software. We have found that an increase of the mass of the hydrogen isotope reduces the boron-hydrogen and carbon-oxygen bond lengths while increasing the boron-carbon distance. In this study, the stability of the adduct has been analyzed in terms of formation energies and B-C bond distances. We have found that the increase of the isotope mass weakens the B-C bond. We tried to give an explanation to this phenomenon based on Lewis acidity concept but it predicted the wrong results. A reactivity model based on the energy differences of borane LUMO orbitals offered a correct explanation to this effect.

Keywords