

Nuclear quantum effects on low barrier hydrogen bonds

Diego Moreno, Sergio Gonzalez and Andrés Reyes

Department of Chemistry, Universidad Nacional - Colombia

A number of symmetric hydrogen bonds have been observed experimentally. However, in some instances, theoretical prediction of these phenomena, with methodologies based on Born-Oppenheimer, may lead to wrong results. In this work, we show how the inclusion of nuclear quantum effects and nuclear-electronic correlation allow for the correct prediction of symmetric of Hydrogen bonded systems. We have carried out the calculations with the APMO code which implements the nuclear orbital and molecular orbital code at the HF and MP2 levels of theory for electrons and hydrogen nuclei.