Conformational Study of Molecular Hydrogen Dimer Derivatives Using ab initio Methods

Hyo Jun Park, Yong Sik Lee, and Sang Joon Kim
Kyung Hee University, Suwon, Korea

The optimized structures of H2 van der Waals dimer and H2-CO2 dimer have been calculated by ab initio methods. The structures of the dimer are studied using Hartree-Fock, and MP2 calculations. The empirical MCG2 higher-level correlation has been suggested by Truhlar et. al. as a successful tool for computational thermochemitsty. Some of the structures of the dimer are studied with density functional methods. The minimum energy and optimized geometry are calculated and compared to the results from conventional methods. The possible dimer structures and their vibrational frequncies are calculated. We conclude that the MCG2 method improves accuracy and costs less.