A QUANTUM CHEMICAL INVESTIGATION OF THE PYRIDINE INTERACTION WITH A MERCURY ELECTRODE

L. Yu. Magnko and W. P. Barabanov

Department of Physical Chemistry, Kazan State Technological University
Karl Marx Str. 68, 420015 Kazan, Russia

A pyridine molecule is a σ- and π-donor of electrons and it can interact via π and N lone pair electrons with a substrate that made it a good model for adsorption and coordination studies on a metal surface. The pyridine interaction with a mercury electrode was examined using Hartree-Fock and DFT quantum chemical methods. The mercury electrode surface was modelled by a planar Hg_7 cluster and pyridine π-ring vertical orientation was considered. The energy profiles of the pyridine adsorption on a mercury electrode have been built. The adsorption energies were found to be ΔE_{ads} = -5.58 kcal mol^{-1} (B3LYP) and ΔE_{ads} = -4.52 kcal mol^{-1} (HF). An orbital populations analysis has shown, that the charge transfer from a metal toward the empty pyridine orbitals is negligible. The obtained results provide new information about the microscopic properties of pyridine adsorbed on mercury surface and will be used to quantum chemical studies of pyridine adsorption on solid electrodes.