SW-P003

Adsorption Selectivities between Hydroxypyridine and Pyridone Adsorbed on the Ge(100) Surface

Myungjin Lee, Hangil Lee*

Department of Chemistry, Sookmyung Women's University, Seoul 140-742, Republic of Korea

The most stable adsorption structures and their corresponding energies of 4-pyridone, 4-hydroxypyridine, 2-pyridone and 2-hydroxypyridine have been investigated by Density Functional Theory (DFT) calculation method and high-resolution photoemission spectroscopy (HRPES). We confirmed that between the two reaction centers of 4- and 2-pyridone, only O atom of carbonyl functional group can act as a Lewis base and thus, O dative bonding structure is the most stable. On the other hand, we clarified that both the two reaction centers (the cyclic N atom and the O atom of hydroxyl functional group) of 4- and 2-hydroxypyridine (tautomers of 4- and 2-pyridone) can successfully function as a Lewis base. Through the interpretation of the N 1s and O 1s core level spectra obtained using HRPES, we could confirm the electronic structures and bonding configurations of these molecules with a coverage dependence on the Ge(100) surface.

Keywords: hydroxypyridine, pyridone, Tautomerism, Ge(100) surface, DFT calculation, Adsorption structure, HRPES.