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Acetic Acid Adsorption and Decomposition on Pt(111): Comparisons to Ni(111)

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Abstract : The interaction of organic molecules with metal surfaces is of interest in numerous technological applications, such as catalysis, bone replacement, and biosensors. Acetic acid is one of the main products of bio-oils produced from the pyrolysis of hemicellulosic feedstocks. However, their high oxygen content makes them unsuitable for use as fuels. Hydrodeoxygenation is a proven technique for catalytic deoxygenation of bio-oils. An understanding of the energetics and control of the bond-breaking sequences of biomass-derived oxygenates on metal surfaces will enable a guided optimization of existing catalysts and the development of more active/selective processes for biomass transformations to fuels. Such investigations have been carried out with the aid of ultrahigh vacuum and its concomitant techniques. The high catalytic activity of platinum in biomass-derived oxygenate transformations has sparked a lot of interest. We herein exploit infrared reflection absorption spectroscopy(IRAS), temperature-programmed desorption(TPD), and density functional theory(DFT) to study the adsorption and decomposition of acetic acid on a Pt(111) surface, which was then compared with Ni(111), a model non-noble metal. We found that acetic acid adsorbs molecularly on the Pt(111) surface, interacting through the lone pair of electrons of one oxygen atomat 90 K. At 140 K, the molecular form is still predominant, with some dissociative adsorption (in the form of acetate and hydrogen). Annealing to 193 K led to complete dehydrogenation of molecular acetic acid species leaving adsorbed acetate. At 440 K, decomposition of the acetate species occurs via decarbonylation and decarboxylation as evidenced by desorption peaks for H_2,CO, CO_2 and CHX fragments (x=1, 2) in theTPD.The assignments for the experimental IR peaks were made using visualization of the DFT-calculated vibrational modes. The results showed that acetate adsorbs in a bridged bidentate ($\mu^2\eta^2$(O,O)) configuration. The coexistence of linear and bridge bonded CO was also predicted by the DFT results. Similar molecular acid adsorption energy was predicted in the case of Ni(111) whereas a significant difference was found for acetate adsorption.

Keywords : acetic acid, platinum, nickel, infared-absorption spectrocopy, temperature programmed desorption, density functional theory

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