

### Kinetic and Spectroscopic Studies of Catalytic Mechanisms

유허남<sup>1,2,†</sup>, 안소진<sup>1</sup>, I. Tyrone Ghampson<sup>1</sup>, S. Ted Oyama<sup>1,2</sup>

<sup>1</sup>The University of Tokyo; <sup>2</sup>Virginia Tech

(kwangnami@gmail.com<sup>†</sup>)

This work focused on the catalytic hydrodeoxygenation (HDO) of the cyclic five-membered ester  $\gamma$ -valerolactone (GVL-C<sub>5</sub>H<sub>8</sub>O<sub>2</sub>) and the kinetic analysis of reaction network of GVL on Ni<sub>2</sub>P/MCM-41.

In addition, a special focus was given to the adsorbed species on the catalyst surface during the reaction were monitored by in situ infrared spectroscopy measurement to support the proposed reaction sequence. The determination of the reaction pathway and the estimation of the reaction constants of each step by a contact time study were investigated. Simulated fitting results to a first-order network showed good agreement with the experimental results. In situ infrared spectroscopy measurements indicated that an intermediate with greater number of CH<sub>2</sub> groups than GVL was formed at reaction conditions, and this gave support for the proposed reaction mechanism, in which the initial reaction led to the production of pentanoic acid which has more CH<sub>2</sub> bonds than GVL.

Overall, the combined kinetic and spectroscopic results give a consistent picture of the mechanism of GVL hydrodeoxygenation on Ni<sub>2</sub>P/MCM-41.