Thana Maihom 2008: Theoretical Study on Reaction Mechanisms of Ethylene Oxide Hydration over H-ZSM-5: An Ethylene Glycol Formation. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Mr. Tanin Nanok, Ph.D. 52 pages.

Stepwise and concerted mechanisms of ethylene oxide hydration reaction within a cluster model covering nanocavity, where the straight and zigzag channels intersect, of H-ZSM-5 have been proposed and investigated by means of the ONIOM(B3LYP/6-31G(d,p):UFF) and embedded-ONIOM(B3LYP/6-31G(d,p): UFF) methods. For the stepwise mechanism, the hydration reaction of ethylene oxide starts from the ring-opening of ethylene oxide by breaking of the C-O bond to form the alkoxide intermediate followed by the hydration of the alkoxide intermediate to produce ethylene glycol as the product of the reaction. The calculated activation energies are computed to be 34.4 and 14.5 kcal/mol for the ring-opening and hydration steps, respectively. For the concerted mechanism, the ring-opening and hydration take place in simultaneously with a small activation barrier of 13.3 kcal/mol. This reaction is suggested as a more economical alternative to the present non-catalytic hydration of ethylene oxide via the concerted mechanism for the production of ethylene glycol, a versatile intermediate in a wide range of applications, and should be of particular interest to industry.

Thana Maihom — Student's signature

Tanin Nanok — Thesis Advisor's signature

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