Jittima Meeprasert 2009: Dehydration of Ethanol to Ethylene over H-MOR Investigated by the ONIOM Method. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Assistant Professor Piboon Pantu, Ph.D. 45 pages.

The conversion of ethanol to ethylene is of particular interest as an alternative method for production of petrochemical feedstock. In this study, two mechanisms, stepwise and concerted, of the ethanol dehydration to ethylene in H-MOR zeolite were theoretically investigated using the ONIOM(B3LYP/6-31g(d,p):UFF) method. The effect of water on the reaction mechanism is also considered because water is commonly found in ethanol produced from biomass. In the stepwise mechanism, the reaction proceeds via dehydration of ethanol to form the surface ethoxide intermediate which is found to be the rate determining step. Then the surface ethoxide is transformed to ethylene. In the concerted mechanism, ethanol dehydrated to ethylene directly without the formation of surface ethoxide. The presence of coadsorbed water is found to reduce the activation energy by 2-3 kcal mol^{-1}. The dehydration of ethanol preferentially takes place via the stepwise mechanism. The first step has an activation energy of 41.2 kcal mol^{-1} and, then, the transformation of ethoxide species to ethylene has an activation energy of 22.2 kcal mol^{-1}. In addition, the presence of coadsorbed water prevents the direct access of the ethylene product to the Brønsted acid site. Therefore, the reverse reaction of ethylene to ethoxide requires a higher activation energy of 34.1 kcal mol^{-1} (compared to 25.1 kcal mol^{-1} without coadsorbed water).

_____ _____ ___ /___ / ___

Student's signature Thesis Advisor's signature