Panida Singra 2011: Structures and Mechanisms Investigation on Etherification of Isobutene with Ethanol Catalyzed by Acidic BEA Zeolite. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Mr. Pipat Khongpracha, Ph.D. 74 pages.

Ethyl *tert*-butyl ether (ETBE) can be considered as a prime candidate for high-octane additive due to its outstanding environmentally friendly properties. ETBE easily mixes with gasoline, to make gasoline burn cleanly and completely, and reduce the vehicle's greenhouse gas emission from the exhaust. In this work, the reaction mechanisms for ETBE production via the etherification reaction of isobutene and ethanol catalyzed by the H-BEA zeolite were investigated by using the full quantum calculations at the M06-2X/6-311+G(2df,2p) level of theory. A catalyzed reaction was proposed to occur via stepwise and concerted reaction mechanisms. The stepwise mechanism starts with the formation of a *tert*-butyl carbenium ion intermediate and then the intermediate reacts with ethanol yielding an ETBE product. The concerted reaction mechanism occurs in one step through the coadsorption of isobutene and ethanol leading to the ETBE formation. Besides the catalyzed reaction, an uncatalyzed reaction was investigated by the bare model system with the same level of theory as the catalyzed reaction. The overall reaction is found to be exothermic and this study gives the calculated reaction energy of -18.4 kcal/mol. The H-BEA zeolite is demonstrated to be an efficient catalyst in the etherification of isobutene with ethanol due to it having a lower energy barrier (8.7 kcal/mol for the concerted reaction mechanism and 9.6 kcal/mol for the stepwise reaction mechanism) as compared to that of the bare model system (53.3 kcal/mol).

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