Kulwadee Theanngern 2013: Quantum Effect on the Reaction Mechanism of Propene Oxide Isomerization in H-ITQ-22: A DFT Investigation. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Mr. Pipat Khongpracha, Ph.D. 60 pages.

The selective isomerization of propene oxide over multi-nanopore zeolite, H-ITQ-22, has been investigated with the M06-2X/6-31G(d,p) method. 14T and 58T quantum cluster covered the intersection 12 membered ring was used to represent the acid site, where T is Si or Al atoms. The reaction were proposed through a stepwise mechanism: the ring opening and the 1,2 hydride rearrangement. Two different pathways were systematically examined leading to the two products, namely propanal and propanone. The ring-opening step of these mechanisms is found to be the rate-determining step with an activation barrier of 24.4 kcal/mol for the propanal and of 38.4 kcal/mol for the propanone. Therefore, the propanal is predicted to be the main product for this reaction. With chemically realistic and well-calibrated models together with an accurate DFT method, our findings clearly demonstrate that H-ITQ-22 zeolite is one of the good catalysts for the selective isomerization of propene oxide for the production of propanal.

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