Oranit Phuakkong 2009: Structure and Reaction Mechanisms of Peptide Formation over Nanostructured Zeolite. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Assistant Professor Piboon Pantu, Ph.D. 48 pages.

The peptide bond formation between two glycine molecules over acidic FAU zeolite was theoretically investigated using the ONIOM2 method. The H-FAU zeolite was modeled with the 120T cluster to include the unique supercage structure of this zeolite. The active region, the 14T cluster of the zeolite acid site, and the reactive molecules were treated with the B3LYP/6-31G(d,p) method. The rest of the 120T model was treated with the UFF force field, to represent the confinement effect of the zeolite pore channel. Three adsorption configurations of two glycine molecules over acidic FAU zeolite, namely Amino-bound, Carboxyl-bound and Hydroxyl-bound, were considered as starting points for the reaction. By comparing the activation energies of various reaction paths, it was appeared that the reaction preferentially proceeds through the concerted mechanism. In the pathway via the most stable adsorption configuration, the Amino-bound, the Brønsted acid site bound strongly with the first glycine molecule but did not involve in the reaction. Therefore, the high activation energy of 51.7 kcal/mol was observed. In the pathway via the Hydroxyl-bound configurations, the Brønsted acid site directly involved in the proton transfer and facilitated the peptide bond formation and, thus, the activation energy was greatly reduced to 11.2 kcal/mol. The results of this study may be helpful for understanding the fundamentals of how peptide formation of amino acid occurs over zeolite.

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