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Thermodynamic Analysis of Transition Metal Oxide Clusters in the Hexane Isomerization Using Quantum Chemical Physics HAEUN LIM, ERIC BAE, RACHEL HUR, Choice Research Group — In this research, the catalyzing ability of transitional metal oxide compounds using a computational chemistry method was assessed in an effort to compute the measures of catalytic ability. Transitional metals, such as Ti, Zn and Pt, have been widely used as prominent catalysts for industrial applications. Catalytic oxidation reactions are crucial for chemical synthesis in pharmaceutical and petrochemical industries. Hexane isomers, such as 2,3 Dimethylbutane and 3-Methylpentane, are formed through the isomerization of hexane, which can be a source of energy by itself. It is a cleaner way to produce with higher efficiency because more branched isomers will release less harmful byproducts. In this research, the catalytic efficiencies of various Ta compounds in the hexane reaction were modeled and explained based on the compounds electron structure. An overview of Tantalum oxide application and the advantages of certain Tantalum oxide among the same groups of metal oxides in the hexane reaction were presented. The Density Functional Theory was used to figure out the best catalyst for the conversion of isomers from hexane, which will advocate the pharmaceutical and petrochemical industries and economy.

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