

## **Investigation of the Dehydration of 2-propanol Over the ZSM-5 Zeolite using NWChem**

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This research investigates the dehydration of 2-propanol within the ZSM-5 zeolite using NWChem and solid state nuclear magnetic resonance. The ZSM-5 zeolite is a catalyst with a unique porous structure mainly used in the petrochemical industries to convert methanol to gasoline and diesel as well as oil refining. Our goal is to understand and verify the results obtained by other research investigating 1-propanol dehydration then investigating the dehydration of the alcohol 2-propanol (isopropyl) using NWChem calculations. We also seek to minimize the structure to decrease the computational cost. Most importantly, we are trying to figure out how aluminum reacts with isopropyl by carving out the cluster of the zeolite around the active site (Al-OH).

### References:

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