Investigate The Dehydrogenation of 2-Propanol Using NWChem

Abstract

This work presents a comprehensive result about Investing the Dehydrogenation of 2-propanol is a crucial process in understanding the mechanisms by which hydrogen is removed from organic compounds to form a new chemical. Relevant data on the dehydrogenation of 2-propanol, propane, water, and enthalpy using different basis sets. The calculations have been done using the Density functional theory (DFT) simulations were used to study the aqueous phase dehydration of 1-propanol over H-ZSM-5 zeolite. The works show how each basis set's enthalpy decreases as the polar valence zeta increases. A quantum chemistry code designed for parallel computers created in 1994 disposes the capability of implementing many energies expression: Hartree-Fock/DFT, MCSCF, etc. The quantum chemistry code has used the methodology and implementation of the steps to investigate the dehydrogenation of 2-propanol using the NWChem.

Keywords: NWchem, 2-Propanol, 1-Propanol, Zeolite, Water, Propene.