

Potential Energy Surface for 1-hydroxy-2-propyl Cation and 2-hydroxy-1-propyl Cation

Chemistry

PowerPoint

Dr. Matthew D. Brynteson (mdbrynteson@liberty.edu)

Holly Tubbs (htubbs@liberty.edu)

Basic

Abstract: This experiment analyzes the possible stable products with their respective energies that are produced when the 1-hydroxy-2-propyl cation and 2-hydroxy-1-propyl cation undergo dissociation to become stabilized. This data will then be used to investigate the most likely product. The motivation for this experiment is to further the previously done research on reactions between propene and OH. Propene is abundant in the atmosphere and reacts with OH regularly. Additionally, propene reactions with OH are of interest for alkene based fuel research as this is an important intermediate in many combustion reactions. This experiment will investigate a potential energy surface for both the 1-hydroxy-2-propyl cation and the 2-hydroxy-1-propyl cation. This shall be done through Gaussian computer calculations. Geometries will be optimized and energies calculated for the stable points along the intrinsic reaction coordinate (IRC). These calculations will be performed at two levels of theory: Second Order Møller–Plesset Perturbation Theory (mp2) and the hybrid density functional theory B3LYP. These will be used along with two different basis sets: 6-311++G(d,p) and 6-31g(d,p). The energies of the transition states will be compared with the lowest energies of the cations in the potential energy surface to calculate likely intermediates and the pathways that could not be observed in experiment. The final data can then be used in the continued research of the propene and OH reactions. Furthermore, the potential energy surfaces for these cations could be accessed for

other avenues of research to assist in understanding the breakdown of such cations as the ones analyzed here.

References: Zádor, J.; Jasper, A. W.; Miller, J. A. *Physical Chemistry Chemical Physics* 2009, *11* (46), 11040–11053.