

Theoretical Study of Pentyl Alcohol Acetylation

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The study of acetylation of alcohols is of great interest by the utility of its products of reaction and is one of the most frequently used transformations in organic synthesis as it provides an efficient means for protecting hydroxyl groups in a synthetic process. A theoretical study of acid acetylation of pentyl alcohol from the analysis of intermediate of the reaction was carried out. Geometries of all species involved in the reaction were made and identified. All of the geometry optimizations were performed and all energies were calculated using the DFT/B3LY method and was adopted the 6-31+G* basis set. Following the same procedure it was identified the geometric parameters and energy of intermediate of reaction. Acetylation of alcohols is a nucleophilic substitution reaction. This reaction can be catalyzed by Brönsted acid. In the mechanism, the acetic anhydride first accepts a proton at the carbonyl oxygen and this change enhances the positive charge on the carbonyl carbon. This facilitates the successive attack nucleophilic of alcohol at the position to form a tetrahedral intermediate, step determinant of the rate of the reaction. Experimental studies and theoretical work agreed that this reaction takes place with the formation of a tetrahedral intermediate. The energy of activation for the reaction was 17.30 kcal/mol. The reaction and the compounds studied are shown in Figure 1, R: C₅H₁₁.

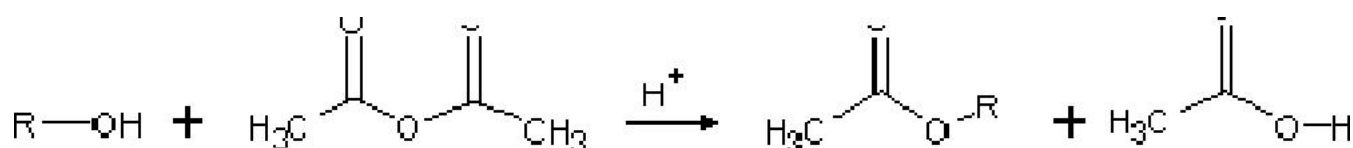
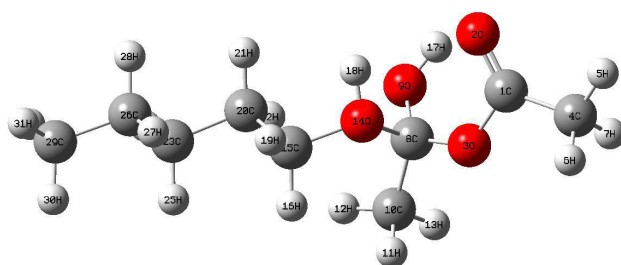


Figure 1 : General Scheme of Acid Acetylation of Pentyl Alcohol



Biography

Silvana Claudia Caglieri is currently working as a professor of Organic Chemistry. He is the Director of the CIQA Research Project – FRC at National Technological University, Argentina.

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