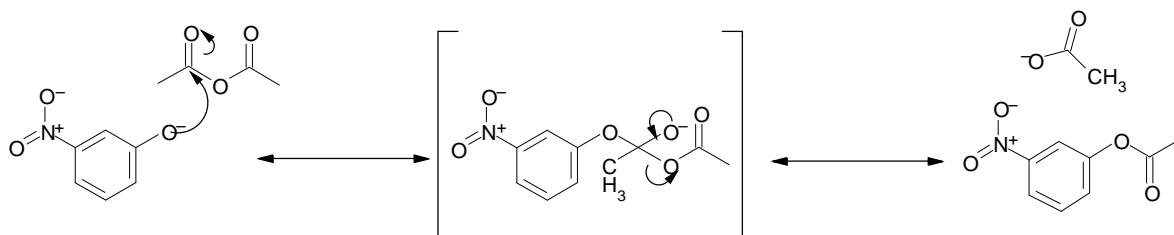


Abstract

It has traditionally been taught that the nucleophilic acyl substitution (NAS) reaction is a two-step process. There is evidence that suggests that this may not be the case. Kinetic studies of the reaction have found that the process does in fact proceed by a concerted or concerted-like process (Ba-Saif, Luthra, Williams, *J. Am. Chem. Soc.* **1987**, 109, 6362). The reaction of acetic anhydride and *m*-substituted phenolates are the particular reaction of study. This research makes use of three computational models to describe the reaction process: B3LYP, MPW1K, MP2. Using MP2, MPW1K, and B3LYP it is possible to determine whether the process is concerted or step-wise. The results for *m*-nitrophenolate show that the process is step-wise when modeled with MPW1K and concerted with B3LYP. The barrier to decomposition of MPW1K between the intermediate and reactants is 1.82 kJ/mol. The barrier to decomposition between the intermediate and products is 7.10 kJ/mol. There was no stable tetrahedral species found using B3LYP. The first transition state for MPW1K had a bond length of 1.78 Å between the phenolate oxygen and anhydride carbon. For the second transition state the bond length was 1.79 Å between the anhydride carbon and anhydride oxygen. The B3LYP transition state was similar to the second transition state of MPW1K with a bond length of 1.84 Å where the bond was breaking between anhydride carbon and anhydride oxygen. Preliminary results from MP2 suggest the mechanism is concerted as well. The results of *m*-nitrophenolate will be used in comparison to other substituted phenols such as *m*-methylphenolate, which has been found to be strictly step-wise thus far.



The tetrahedral intermediate or transition state