Nucleophilic Acyl Substitution of Acetic Anhydride with Substituted Phenolates: MP2

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This project is a computational investigation of the nucleophilic acyl substitution, NAS, reaction mechanism using the MP2/6-31+G** level of theory. There is some disagreement as to whether these reactions occur in a concerted or a stepwise process. We are hoping to show that NAS reactions between weak nucleophiles and molecules that contain a good leaving group will occur in a concerted step, while those with a stronger nucleophile, will proceed through a two step process. The systems that we will be investigating are *m*-nitropheol (weak nucleophile) reacting with acetic anhydride and *m*-methylphenol (stronger nucleophile) reacting with acetic anhydride. We hope to show that the reaction involving *m*-nitrophenolate is concerted, while the reaction involving the *m*-methylphenol is not. Preliminary results show that as expected the *m*-methylphenolates react in a two-step mechanism as shown in the figure below.