Effects of SMD and SM8 Solvation Models on the Nucleophilic Acyl Substitution Reactions of *m*-Methyl and *m*-Nitrophenol in Acetic Anhydride

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The aim of this research is to come closer to fully understanding the capability of three solvation methods (PSM, SMD, and SM8) to model the effect of solvent on the reaction of various phenols with acetic anhydride. Previous results using the M3LYP, MPW1K, and MP2 levels of theory revealed that some nucleophilic acyl substitution reactions occur in the gas phase with an isolatable tetrahedral intermediate while others do not. These results led to the use of another computational method known as M06-2X. This report uses the M06-2X density functional with the SM8 and SMD solvation methods to study the reactions of *m*-methyl and *m*-nitrophenol with acetic anhydride. Using the 6-31+G** basis set, the acid dissociation constants for six phenols and two carboxylic acids were calculated and compared to literature values. Using the same basis set, reaction energy profiles for *m*-methylphenol and *m*-nitrophenol were determined to study the progression of each reaction and to aid in better understanding the nucleophilic acyl substitution reaction mechanism by first finding the lowest energy conformer of each molecule. Preliminary data indicates that the reaction of *m*-methylphenol contains two transition states and an isolatable intermediate, while the reaction of *m*-nitrophenol contains only one stable transition state.