

## Solvent Effects on the Reaction of *m*-Methylphenolate with Acetic Anhydride

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The nucleophilic acyl substitution reaction process between *meta*-substituted phenolates and acetic anhydride has been suggested to proceed as either concerted or step-wise. The first involves only one transition state between reactions and products, while the latter includes two high energy transition states and the formation of a relatively stable tetrahedral intermediate. Some experimental evidence has preferred the concerted process but nothing conclusive has been found (Ba-Saif, Luthra, Williams, *J. Am. Chem. Soc.* **1987**, 109, 6362). Previous research in our group has used the 6-31+G\*\* basis set and B3LYP computational method to study this reaction process in the gas phase focusing on the electronics effect of substituents; *m*-nitrophenolate gives a concerted process while *m*-methylphenolate is step-wise. It is the goal of this research to determine how SM8 and SMD solvation models affect the step-wise reaction profile of *m*-methylphenolate with acetic anhydride in the aqueous phase. Preliminary tests using both models tracked solvation effects on three structures optimized in the gas-phase: transition state one, a putative tetrahedral intermediate, and transition state two. Calculations on these complexes using SMD and SM8 show a linear downward trend in energy with transition state two 12.4 kJ/mol more stable than the tetrahedral intermediate. Further research with optimization in the aqueous phase will be necessary to clarify these findings.

