Investigating the Nucleophilic Acyl Substitution Reaction using the Polarizable Continuum Model

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This project is part of a larger project examining the nucleophilic acyl substitution (NAS) reaction, specifically the reactions between *m*-nitro and *m*-methylphenol and acetic anhydride. There is disagreement as to whether NAS reactions proceed through several transition states, or if they take place in a concerted process. This particular project makes use of the polarizable continuum model for solvation. Built into the project, is an evaluation of the ability of various solvation models to accurately predict reaction energies. The goal is to create reaction energy profiles for the reactions of the most energetically favorable conformers of the substituted phenolates and acetic anhydride. By finding the geometries and energies of isolatable transition states and tetrahedral intermediates we hope to understand when NAS reactions occur in a concerted or a stepwise process. Preliminary results indicate that, while there is a large energy difference between the energies of the first transition state and the tetrahedral intermediate, the activation energy for the second step is relatively small, for example see figure below.