

Effect of Solvation with PCM on the Activation Energies of Acetylation of *m*-Methylphenolate

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The reaction of acetic anhydride and various phenol and phenolates has previously been thought to occur by a two-step process. Previous work has shown that in the gas phase some phenol and phenolates react by a concerted (one-step) process. When looking at phenols and phenolates in the gas phase, the molecules were isolated; thus, they were not interacting with the environment. In reality, this reaction occurs in water. This study examines the effect(s) of aqueous solvation using PCM models on the reaction pathway of *m*-methylphenolate. The effect of aqueous solvents on these reactions was studied using the 6-31+G** basis set and the B3LYP method to see if water stabilizes the tetrahedral intermediate of *m*-methylphenolate relative to the transition states leading to and away from it; if stabilization occurs in solvent, it may suggest that the inflection point of nitrophenolate can be stabilized into an intermediate in a two-step process. To assess the effectiveness of PCM⁷ solvation models (PCM, IPCM, SCIPCM, and CPCM), the acid dissociation constants and relative energies will be calculated computationally using both gas and aqueous phase geometries in Gaussian '09. Once best way to account for the effects of solvent is determined, this information will be used to study reaction energy profile for the reaction *m*-methylphenolate. Solvent's effect on the relative energy and geometries of *m*-methylphenolate will be observed by looking at the energies of the reactants, transition states, intermediates, and products to construct an energy diagram to model the reaction.

