Computational Investigation of the Nucleophilic Acyl Substitution Reaction of *m*-Methyl and *m*-Nitrophenols with Acetic Anhydride in the Gas Phase

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The Nucleophilic Acyl Substitution reaction of *m*-methyl and *m*-nitrophenols with acetic anhydride have previously been studied using the B3LYP, MP1WK and MP2 methods and the 6-31+G** basis set.. It has been decided a relatively new method, the M06-2X, should be used. In the past the methods have been used with the 6-31+G** basis set as it was most appropriate but this has not been tested with the new method. To determine the most appropriate basis set this basis set and three others (6-31+G*, 6-311+G* and 6-311+G**) were used to calculate several gas phase acidities and checked with the experimental values to determine the most accurate. The 6-31+G** basis set was determined to be again the most appropriate basis set and used to determine the reaction profiles of the NAS reactions of *m*-methyl and *m*-nitrophenols with acetic anhydride. This method was then used to determine the transition states of the reactions. This was done by taking the most stable conformers of the tetrahedral intermediates and preforming QST3 calculations in Gaussian '09. Activation energies of X-Y kJ/mol have been found.