Determining the energy profile of the reaction of *m*-fluorophenol with acetic anhydride

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The reaction of acetic anhydride with substituted phenolate ions is suspected to proceed by a concerted mechanism, with bond formation between the phenolate oxygen and bond breaking between acetate groups occurring in one step. Experimental evidence does not clearly show whether the reaction occurs with one or two steps, so the reaction was studied by a computational approach. The reaction of *m*-fluorophenolate with acetic anhydride was modeled using MPW1K/6-31+G** and B3LYP/6-31+G**. The energy profile of the reaction was determined by stepping bond length of the phenolate-carbonyl bond and the carbonyl-acetate bond, with smaller steps used near energy maxima. The geometry of the maxima was optimized to the transition state and confirmed as a transition state by frequency and IRC analysis. Two conformers of the tetrahedral intermediate were found using MPW1K and B3LYP. The barrier heights of decomposition of the conformer with the lowest overall activation energy were determined. MPW1K calculation found two transition states and a tetrahedral intermediate. The barrier height for decomposition of the tetrahedral intermediate to phenolate and acetic anhydride was determined to be 2.8 kJ/mol and the barrier height proceeding to products was determined to be 6.5 kJ/mol using MPW1K/6-31+G**. The barrier height for decomposition of the tetrahedral intermediate to products was determined to be 23.2 kJ/mol using B3LYP/6-31+G**. No barrier was found for decomposition of the tetrahedral intermediate to reactants using B3LYP/6-31+G**.