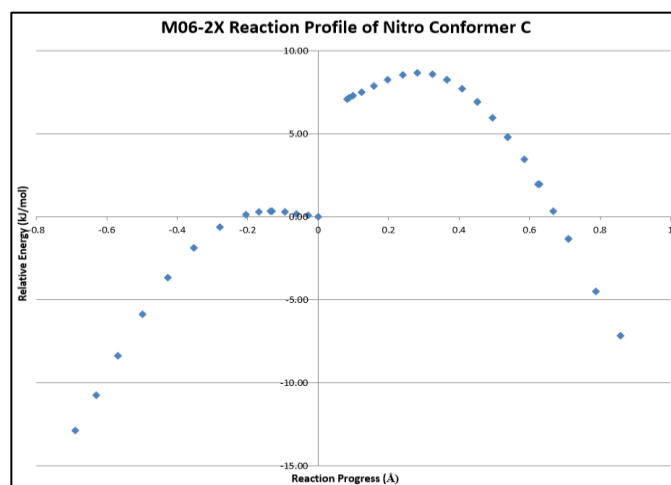
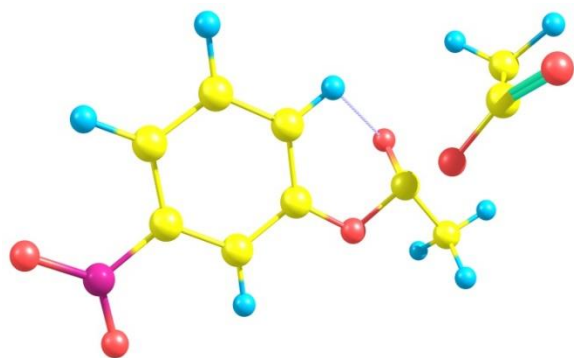


Investigations into the Mechanisms of Nucleophilic Substitution Reactions with M06-2X

Phuc Vo, and Justin Houseknecht
Department of Chemistry, Wittenberg University
Springfield, OH

This computational project investigates the nucleophilic acyl substitution (NAS) reactions between acetic anhydride and either *m*-methylphenolate or *m*-nitrophenolate. One of the main goals of this investigation is to computationally model the kinetics of these NAS reactions in both gas and rigid aqueous phase in order to determine whether they occur through step-wise or concerted processes. This is achieved mainly through studying transition state energies, reaction profiles, as well as changes in partial charge distribution as the reactions progress. The project is performed with Gaussian '09 using the M06-2X density functional method and the 6-31+G** basis set, which, according to previous work on this topic, will most accurately describe these reactions. Results obtained from several conformers so far have revealed that the general reaction profiles vary significantly between conformers across both types of phenolates, and that both step-wise and concerted mechanisms have been observed within each phenolate group. However, a general trend is seen, and is expected, where the *m*-nitro reaction is concerted and the *m*-methyl reaction is step-wise. By comparing these results with those produced by SMD solution phase investigations as well as those using the MP2 method, we hope to shed more light on the mechanistic properties of these NAS reactions.



An *m*-nitrophenolate tetrahedral intermediate (left) and the appropriate reaction profile generated with Gaussian '09