

# Nucleophilic Acyl Substitution of Acetyl Cyanide with Cyanide

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Nucleophilic acyl substitution reactions are typically described as occurring via a tetrahedral intermediate (associative pathway, below). A dissociative pathway is also known to occur when a weak nucleophile reacts with a carbonyl containing an excellent leaving group. This project aims to examine the space between these two extremes and determine whether a viable concerted pathway exists. Gas phase acidity calculations of several common leaving groups / nucleophiles found the M06-2X/aug-cc-pVDZ and MP4/aug-cc-pVTZ//MP2/aug-cc-pVTZ methods to be most appropriate for these studies. These methods were used to calculate the energies of all reactants, intermediates, and products in the identity exchange reaction of acetyl cyanide with cyanide. Transition states were found using QST3 calculations. All structures were confirmed via frequency calculations and transition states were further confirmed by IRC analysis.

