

## Abstract

An accurate understanding of any reaction mechanism is obtained by vividly understanding its minima, intermediates, transition states along with the complete reaction pathway. Experimental studies often need computational collaboration to provide an affirmation for any chemical reaction. Where one part of the thesis focuses on developing an algorithm for finding guess structures of transition states, the second part is about computational study of an organic reaction. Using the vibrational description of pre reaction complex and product, an harmonic oscillator approximation is created at each minimum. The region where these potentials intersect provide an approximation for the transition state structure of the corresponding reaction. The second problem is concerned with the computational study of Nucleophilic Heterocyclic Carbene catalysis. In the presence of these NHCs, under aerobic conditions, aromatic aldehydes have been experimentally known to undergo esterification with boronic acids. Using first principles, we analyse the mechanism for this reaction.