EASTERN MICHIGAN UNIVERSITY

A Computational Exploration of the Steroselective Synthesis of Substituted Pyrrolidines

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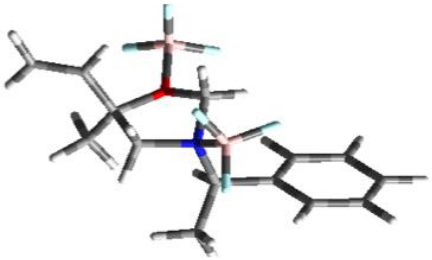
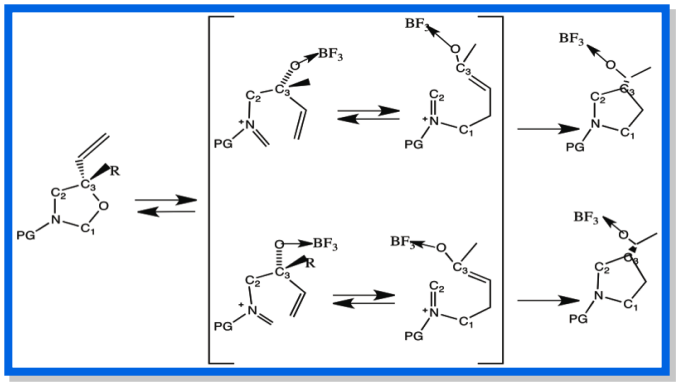
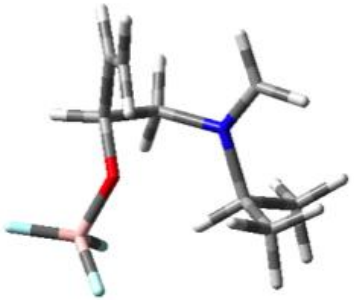
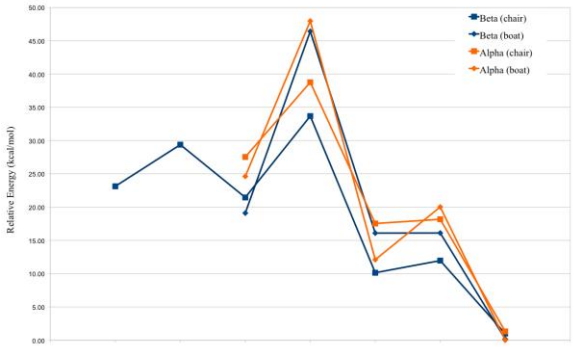






- Goals: to explore
  1. The ring-opening reaction of oxazolidines
  2. The influence of substituent size on the aza-Cope – Mannich reaction
  3. Potential erosion of stereoselectivity via C-C bond rotation



- Results
  1. Lewis acid coordination at both of oxazolidine's nucleophilic sites leads to epimerization and loss of stereoselectivity
  2. Smaller substituents lead to poorer stereoselectivity
  3. Iminium cations with smaller substituents are more likely to undergo C-C bond rotation and subsequent loss of stereoselectivity