General Information About Claisen Rearrangements

- The reaction is a pericyclic reaction.
- 398 K is the temperature at which the experiment was conducted.
- Very versatile and powerful reaction for synthesis.

Curtin-Hammett Principle

\[ \text{[Pa]/[Pb]} = \exp[-(G_{\text{a}} - G_{\text{b}})/RT] \]

Transition States

Results Summary

- Remarkably good agreement between theory and experiment in many of the phenyl substituent results.
- B3LYP did not agree with experiment for cases 3 & 5.
- Not as good agreement between theory and experiment in the n-propyl substituent results.

Computational Details

- All stationary points were verified by calculating second derivatives at the stationary points. In particular, all transition states had exactly one imaginary frequency. Transition states were connected to particular reactants and products via Intrinsic Reaction Coordinate calculations.

Future Work

- Use another method, RPA, on the phenyl substituent cases.
- Further explore the cases that did not agree well.

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