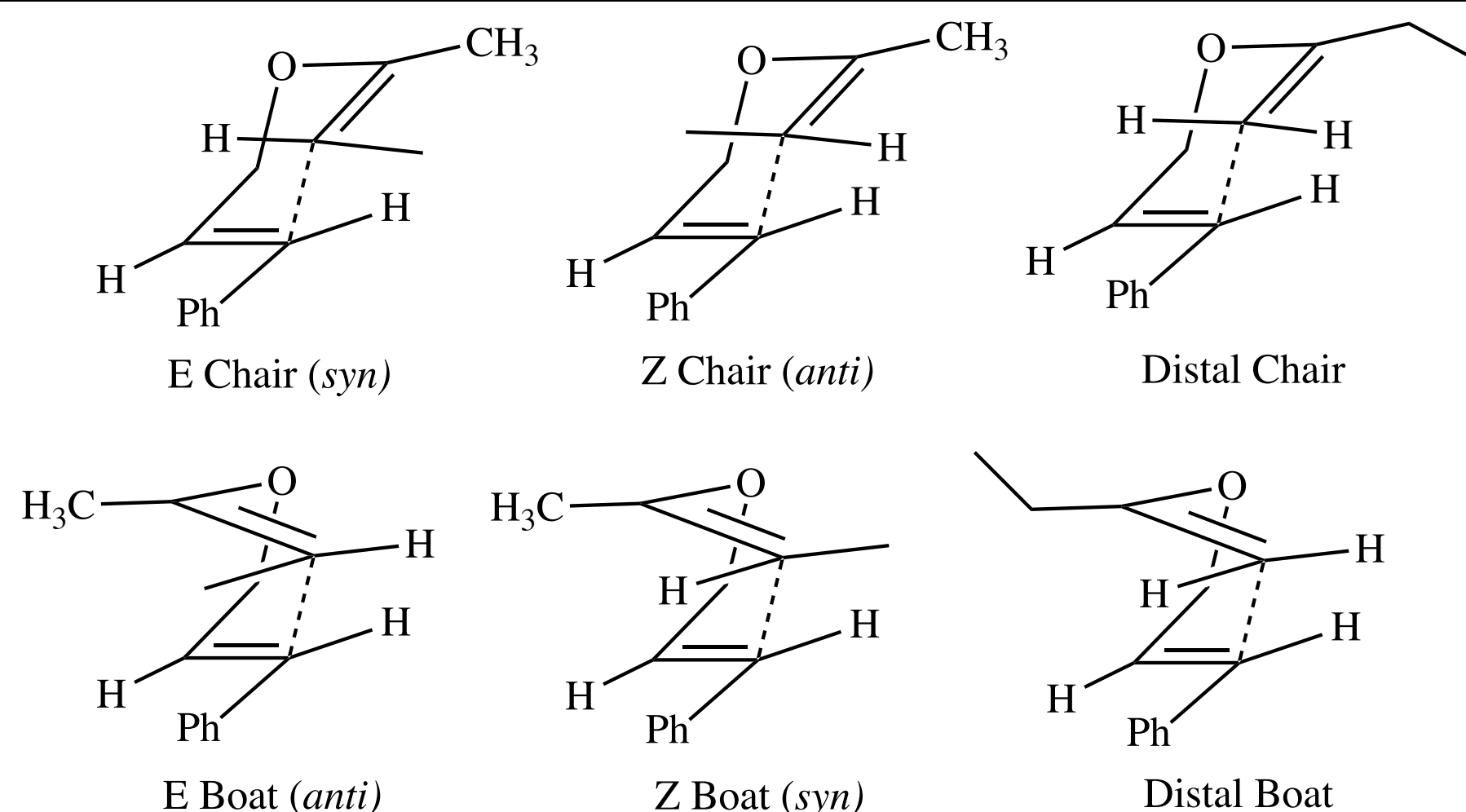




Comparing Density Functional Theory with Experimental Results of Claisen Rearrangements

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The Claisen rearrangement is a very versatile and powerful reaction for synthesis. The Claisen reaction can go through either the chair or boat transition states.

Density Functional Theory is the strategy of utilizing the electron density of a system to calculate the energy instead of dealing with the complications of a wave function. It is useful because it is much more computationally efficient than wave function approximations.

This summer, we ran computations on the transition states of Claisen rearrangements with various substituent groups. We found that the theory agreed with experiment in most of the cases but there were some in which the theory was not sufficiently accurate. We are going to further investigate these cases.

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