

Ph.D. THESIS DEFENSE

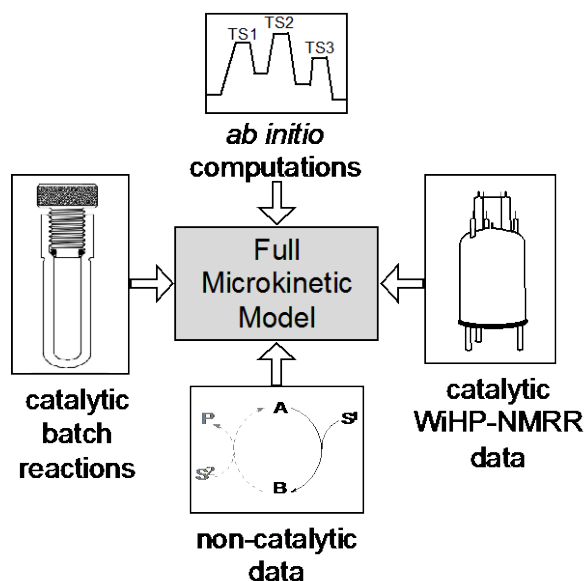
Kinetic and Mechanistic Studies of Rh(Bisdiazaphospholane)-Catalyzed Asymmetric Hydroformylation

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Under the Supervision of Prof. Clark R. Landis

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3:00 p.m. in Room 9341



Hydroformylation of alkenes to generate aldehydes is one of the largest scale homogeneously catalyzed reactions in chemical industry forming primarily the achiral, linear aldehyde. The 3,4- bis(diazaphospholane) (BDP) class of ligands developed by Landis and coworkers exhibits high selectivity and rates for the asymmetric variant of this reaction. The goal of this work is to better understand the high selectivity in rhodium BDP-catalyzed hydroformylation and to develop a robust kinetic model that can predict rate and selectivity under any reaction conditions. Theoretically, *ab initio* computations allow for modeling under any conditions, but in practice, they are not accurate enough to be used in a microkinetic model. For example, these high-level computations predict AHF of styrene to favor the linear product and take years to achieve full conversion, but experiments show a branched-selective reaction reaching completion on the order of minutes to hours. Therefore, the goal of this work is to adjust the calculated energies of transition states and intermediates using various types of experimental data to obtain an accurate, empirically-adjusted surface.