Vita

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Universities Attended:

University of New Brunswick (2015)
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1,2-Asymmetric Induction in Carbonyl Compounds – A Computational Study

UNIVERSITY OF NEW BRUNSWICK

THESIS DEFENCE AND EXAMINATION

in Partial Fulfillment

of the Requirement for the Degree of
Master of Science

by

Jeffrey D. Retallick

in the Department of Chemistry

U.N.B., Fredericton, N.B.

Thursday, November 7th, 2019
2:30 p.m.

Toole Hall, Room 303

Examining Committee

Dr. Ghislain Deslongchamps	Supervisor
Dr. Rodney Cooper	Internal Examiner
Dr. Ben Newling	Int-Ext Examiner
Dr. Gilles Villemure	Chair of Oral Examination

Abstract

In asymmetric synthesis, it is important to reliably predict the major stereoisomeric product of a reaction. One such reaction is the nucleophilic addition to a carbonyl compound featuring an adjacent chiral carbon. Several reaction models exist in literature to predict the facial selectivity of these reactions. These models provide simple visual drawings to quickly predict the major product of such a reaction without requiring exhaustive quantum mechanical calculations. These models are used on a daily basis, and some models perform better than others, making it valuable to investigate which ones are the most effective. For the first time in this thesis, high-level computations have been performed on all of the literature models to verify the efficacy of these models. The results of this thesis offers a definitive answer that the Felkin-Anh and Wintner models are the most effective, and that bent bond theory offers an interesting insight on the mechanics of these reactions.