Notice of the Final Oral Examination
for the Degree of Master of Science

of

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BSc (Vancouver Island University, 2016)

"Automation of Reaction Monitoring"

Department of Chemistry

Thursday, February 21, 2019
1:00 P.M.
Elliott Building
Room 305

Supervisory Committee:
Dr. J. Scott McIndoe, Department of Chemistry, University of Victoria (Supervisor)
Dr. Dennis Hore, Department of Chemistry, UVic (Member)

External Examiner:
Dr. Reuven Gordon, Department of Electrical and Computer Engineering, UVic

Chair of Oral Examination:
Dr. Bonnie Leadbeater, Department of Psychology, UVic

Dr. David Capson, Dean, Faculty of Graduate Studies

Abstract

Automation plays an integral role in our daily lives. From transportation to agriculture, we rely on robots and programs to assist in accomplishing tasks. Chemistry is no except with the deployment of high throughput screening and the recent machine-led reaction discovery, there is increased interest to integrate artificial intelligence and robotics beyond medicinal and synthetic organic chemistry. The addition of automation to mechanistic studies can improve the method in which reactions are understood experimentally and fundamentally.

Chapter 1 introduces the basics of reaction chemistry. As we are interested in *how* the reaction occurs, for this work, there is a natural bias towards understanding kinetic behaviour. Chronograms obtained through mass spectrometry facilitate understanding of kinetics. The introduction of mass spectrometry in this chapter establishes the foundation of this technique for the subsequent experimental chemistry chapters.

Chapter 2 investigates the reduction and subsequent oxidation of titanocene, generating a complex mixture of oxidized products. During this investigation, an interesting and rare methyl abstraction event occurred that led to the deuterium label study to understand a radical-based oxo-titanium reaction. This was made possible by Pressurized Sample Infusion Electrospray Ionization Mass Spectrometry (PSI-ESI-MS) coupled with a smartphone colorimetry technique developed herein known as ColorPixel.

In Chapter 3 we explore the integration of machine learning with reaction monitoring. The attempt to classify reaction roles based on kinetic traces was done to automate the process of identifying important species in a reaction. Often there is a large amount of data from a PSI-ESI-MS experiment, but it is time-consuming to pick out the most important species. Implementing machine learning for reaction role classification can ease this process from taking three months to accomplish to one day. This chapter also outlines the development of Kendrick, an automated reaction sampler. Combined, these tools have the potential to impact reaction monitoring through robotic assistance and can speed up the process of reaction quantification through automated processing platforms to handle the streams of data.

Chapter 4 starts with the implementation of a lightweight mass spectrometry library, Spectrally, that is suitable for any developers using python. This platform establishes a firm foundation that can enable developers to build complex programs using simple code. This chapter also describes the collaboration project PythoMS and the development process for this framework. In addition to the framework, the chapter also describes the development of two pieces of processing software: Sinatra – a cloud-ready EDESI processing platform, and AutoMRM – a cloud-based Multiple Reaction Monitoring method development web application.