University of Victoria | Graduate Studies

Notice of the Final Oral Examination for the Degree of Doctor of Philosophy

of

LARS YUNKER

BSc (University of British Columbia, 2012)

"Real-Time Mass Spectrometric Anaylsis of Catalytic Reaction Mechanisms"

Department of Chemistry

Thursday, April 13, 2017
9:00 A.M.
David Turpin Building
Room A136

Supervisory Committee:
Dr. Scott McIndoe, Department of Chemistry, University of Victoria (Supervisor)
Dr. Alexander Briggs, Department of Chemistry, UVic (Member)
Dr. Dave Berg, Department of Chemistry, Uvic, (Member)
Dr. Kathryn Gillis, School of Earth and Ocean Sciences, UVic (Outside Member)

External Examiner:
Dr. Cathleen Crudden, Department of Chemistry, Queen's University

Chair of Oral Examination:
Dr. Ian Putnam, Department of Mathematics and Statistics, UVic

Dr. David Capson, Dean, Faculty of Graduate Studies

Abstract

Mass spectrometry was used to study two disparate transformations: in an applied project, the supposed degradation of perfluorooctanesulfonate (PFOS); and in a fundamental study, the Suzuki-Miyaura (SM) reaction was investigated in detail. The first investigation revealed that published methods to degrade PFOS were ineffectual, with apparent decreases being associated with adsorption onto available surfaces. In the Suzuki-Miyaura reaction, a dynamic series of equilibria were observed, and there is no direct evidence of a single pathway. Instead, there appear to be two mechanisms which are active in different conditions (one fluoride, one aqueous). Studies were initiated into the related SM polycondensation reaction and the hydrolysis of aryltrifluoroborates, the former indicating a step-growth mechanism, and the latter indicating a dynamic series of equilibria which is very sensitive to experimental conditions. Processing and interpretation of mass spectrometric data was a significant part of all of these projects, so a python framework was developed to assist in these tasks and its features are also documented herein.