University of Victoria | Graduate Studies

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

of

YANG WU

BEng (Central South University, 2014)

"Reaction Monitoring Using Real-time Methods"

Department of Chemistry

Tuesday, July 26, 2016
1:00 P.M.
Elliott Building
Room 305

Supervisory Committee:
Dr. Scott McIndoe, Department of Chemistry, University of Victoria (Supervisor)
Dr. David Harrington, Department of Chemistry, UVic (Member)

External Examiner:
Dr. Jason Hein, Department of Chemistry, University of British Columbia

Chair of Oral Examination:
Dr. Mantis Cheng, Department of Computer Science, UVic

Dr. David Capson, Dean, Faculty of Graduate Studies

Abstract

Electrospray ionization mass spectrometry (ESI-MS) is a powerful method to monitor organometallic reactions. It is fast at generating each spectrum, soft to fragile organometallic and sensitive to detect intermediates in low concentration. When coupled with the pressurized sample infusion (PSI) that helps to continuously inject reacting solution to the MS, both an inert-gas atmosphere and real-time reaction monitoring can be achieved. Also, collision induced dissociation of MS can be used to probe the relative binding affinity of phosphine ligands in ruthenium complexes.

PSI ESI-MS can be coupled with Fourier transform infrared spectroscopy (FTIR) to monitor the rhodium-catalyzed hydroacylation simultaneously. This technique expands the dynamic range to 5 magnitudes.

The effect of mass-transfer in heterogeneous hydrogenation of charge-tagged alkyne was also studied by PSI ESI-MS. In this study cross area, stirring effect, catalyst loading and hydrogen concentration were considered and tested. Also in the study an interesting finding reveals in heterogeneity of the solution.

Relative binding affinity of different phosphine ligands was attained from comparing the relative intensity of fragmentation products from MS/MS. And the phosphine ligand substitution reaction real-time monitored by the ESI-MS. A competitive dissociative substitution mechanism was proposed and testified by the simulation and modeling of COPASI.