University of Victoria | Graduate Studies

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

of

ALAN AN JUNG WEI

BSc (McGill University, 2017)

"Mass Spectrometric Analysis of the Reactivity of the Trityl Cation"

Department of Chemistry

Thursday, April 24, 2019
9:30 A.M.
Elliott Building
Room 305

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

External Examiner:
Dr. Heather Buckley, Department of Civil Engineering, UVic

Chair of Oral Examination:
Dr. Sally Brenton-Haden, Department of Education Psychology & Leadership Studies, UVic

Dr. David Capson, Dean, Faculty of Graduate Studies

Abstract

Ever since its accidental discovery in the 70s, methylaluminoxane, MAO, has been a popular and widely used activator in olefin polymerization. Hydrolysis of trimethylaluminum, Me_3Al, produces MAO, an aluminum-, oxygen-, and methyl containing oligomer. Polyolefins have become one of the most produced polymers, where MAO-activated single-site catalysts are responsible for the synthesis of polymers with highly defined structures.

The detailed structure of MAO however, remains a mystery. In order to thoroughly understand the reactivity of MAO, knowing more about it is essential. Electrospray ionization mass spectrometry (ESI-MS) has proven to be a useful technique for studying catalysts and their activation chemistry. It has been shown that MAO is best thought of as a source for the highly reactive and Lewis acidic dimethylaluminum cation, $[Me_2Al]^+$. Synthetically, this ion is accessible via the reaction between trityl tetrakis(pentafluorophenyl)borate, $[Ph_3C]^+[B(C_6F_5)_4]^-$ and trimethylaluminum, and this reaction was investigated in detail. A new reaction, substitution of H for CH_3 onto the phenyl ring of the trityl carbocation, $[Ph_3C]^+$, was detected and found to be general for all trialkylaluminums studied.

All instruments with detectors are prone to saturation at high concentration and mass spectrometers are no exception. Despite the advantages that ESI-MS offers, saturation can be one of the main obstacles in terms of the accurate quantification of species.

This thesis tackles saturation issues in ESI-MS explicitly, because relatively high concentrations were necessary in order to keep unwanted decomposition reactions to a minimum. By detuning various parameters that allows troubleshooting this issue, data that better reflects the reality and the corresponding quantification of species is obtained. With the optimal settings of parameters, quantitative studies and the reactivity regarding the addition of trimethylaluminum, Me3Al, to the trityl carbocation $[Ph_3C]^+$ can be better understood.