University of Victoria | Graduate Studies

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

of

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BSc (Tianjin Medical University, 2014)

"Selective Analysis of Petroleum Fractions by Mass Spectrometry"

Department of Chemistry

Friday, January 27, 2017
9:00 A.M.
Cornett Building
Room B143

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

External Examiner:
Dr. Jay Cullen, School of Earth and Ocean Sciences, UVic

Chair of Oral Examination:
Dr. Boualem Khouider, Department of Mathematics and Statistics, UVic

Dr. David Capson, Dean, Faculty of Graduate Studies

Abstract

Electrospray ionization mass spectrometry (ESI-MS) is a fast and sensitive technique that is ideal for detecting low concentration species of interest within complex mixtures. Because ESI-MS simply transfers charged species to the gas phase, only ions pre-formed in solution are visible. Accordingly, the charged tag, 3-(4-(bromomethyl)benzyl)-1-methylimidazolium hexafluorophosphate, was designed and synthesized to allow selective detection of phenols in petroleum fractions. Pressurized sample infusion (PSI) was optimized and used for time dependent analyses. PSI ESI-MS was applied to measure O-alkylation of the phenol species leading to rate information about the overall reaction along with dynamic information about reaction progress. The relative intensity of the charged tag was used to determine the presence of phenols in different petroleum fractions.

Other derivatization methods in petroleomics were also explored. 1-[3-(Dimethylamino)propyl]-3-ethylcarbodiimide methiodide (EDT) derivatization followed by PSI ESI-MS analysis was applied for the selective measurement and identification of naphthenic acids in petroleum fractions. The reactions of standard naphthenic acids and EDT were studied by PSI ESI-MS to assess the efficiency of EDT and the rate of reactions.

The same petroleum fractions were analysed by cold Electron ionization (Cold EI) gas chromatography-mass spectrometry (GC/MS) and classical EI GC/MS. The combination spectra from the subtraction from cold EI spectra to classical EI spectra provide us a new dimension to cold EI analysis of complex matrices. Meanwhile, a Python program was written to rapidly screen cold EI GC/MS data for routine tasks, such as retention times comparison on different instrument parameters for single petroleum sample and spectra comparison on the same retention time for different petroleum samples.