Energy, Petroleum & Biofuels Interest Group Workshop:
Use of Mass Spectrometry to Overpower Complexity of Biofuels and Petroleum
Presiding: Patrick Hatcher and Lateefah Stanford
Estimated attendance: 75
Date: 06-16-14

Presenter 1: Wolfgang Schrader
Title: Hyphenated Methods for Petroleum

Synopsis:

1. Investigation of ion mobility with mass spectrometry to investigate:
   a. Isomers
   b. Differentiate how subtle chemistries isomers play roles in:
      i. Polymerization
      ii. Fouling (1, 2 vs 2,4 substitutions, island vs archipeligo asphaltenes, 5- vs 6-carbon ring structures)
   c. Applications for DOM characterization: Lignan vs CRAM (carboxy rich allycyclic material), terrestrial vs marine material, carbon cycling.

Presenter 2: Sunghwan Kim
Title: Advances in FTMS for the Petroelum Field
Synopsis:

1. There are ~30-40 papers published annually on the subject of petroleum HRMS.
2. Current progress in instrumentation and data analysis enhancements include:
   a. Dynamically harmonized cell for enhanced resolution
   b. PCA software
   c. 3D DBE and Van Krevelen Plots for data analysis
3. Current challenge: Structural elucidation by IMS paired with FTMS:
   a. Propose structures of an ion from its elemental composition determined by FTMS analysis.
   b. Calculate the collision cross-section for the proposed structures.
   c. Compare the calculated collision cross-section with the experimental collision cross-section determined by ion mobility analysis.
4. The speaker is an organizer for the PACIFICHEM (International Chemical Congress of Pacific Basin Societies) meeting December 15-20, 2015 and welcomed submissions for abstracts to the analytical section.

Presenter 3: Yury Kostyukevich
Title: New Approaches for NOM Characterization

Synopsis:

1. Discussion on H/D and $^{16}O/^{18}O$ exchange capability in an ESI source for structural characterization of natural organic matter. The ESI source was saturated with deuterium or ^{18}O to prevent back exchange.
2. Experiments conducted for structural differentiation of labile and non-labile oxygen (i.e. esters) and hydrogen in an ESI source include:
   a. H/D exchange of dissolved organic matter by $D_2^{16}O$ vapors.
   b. Acid catalysed backbone H/D exchange of dissolved organic matter by $D_2^{16}O$ with TFA @ 90 C
   c. Acid catalysed backbone $^{16}O/^{18}O$ exchange of dissolved organic matter by $H_2^{18}O$ with TFA @ 90 C

Presenter 4: Pat Hatcher
Title: Use of 2D correlations for data analysis

Synopsis:

1. Plotting FT-ICR data (H:C, O:C, S:C, KMD, and Mass) vs FT-IR and NMR spectra to map correlations and infer structure in a similar manner that 2D NMR spectra are used for structural correlations.