PROTON AFFINITY-BASED KENDRICK PLOTS FOR CLASSIFICATION OF OIL SAMPLES: POTENTIAL IN SOURCE CHARACTERIZATION

Mahsan Miladi¹, Behrooz Zekavat¹, James Clark¹, and Touradj Solouki¹
Vagif Mejid oglu Farzaliyev², Pervin Sh. Mammodova², and Elbay R. Babayev²
¹Department of Chemistry, 5706 Albert Hall, University of Maine, Orono, ME 04469-5706
²Institute of Chemistry of Additives/Azerbaijan National Academy of Sciences, Baku, Azerbaijan

INTRODUCTION

The utilization of ion-ion reactions, ions, and ions/molecules in analytical chemistry research provides an effective analytical tool for the discrimination of organic compounds. The use of ions/molecules for the determination of organic compounds, such as di-isopropyl ethylamine (DIAE), has been widely used in mass spectrometry (MS) studies because of its high mass resolving power and mass measurement accuracy capabilities. FT-ICR mass spectra of crude oil samples contain several peaks, indicating the presence of a wide range of organic compounds.

EXPERIMENTAL

Sample Preparation:

The sample was prepared by dissolving 1.0 g of sample in 1 L of toluene (Fisher Scientific, Pittsburgh, PA), which was further diluted to total volume of 950 µL. The solution was then analyzed for both Kendrick mass defect and PA Kendrick plots.

Data Analysis:

The Kendrick mass defect of a compound is defined as the difference between the nominal mass and the Kendrick mass. Kendrick mass defect vs. Kendrick nominal mass is a graph that provides additional dimensions for successful MS analysis.

RESULTS and DISCUSSION

A) Proton Affinity (PA)-Based Kendrick Plots: Classification of Organic Compounds in a Complex Mixture Based on Both Kendrick Mass Defect and PA Kendrick plots can be used to distinguish between different compounds in a sample. The PA Kendrick plots can be used to identify compounds with similar Kendrick mass defects but different PA values.

B) Experimental Observations for the Reaction between a Petroleum Sample and Diisopropylethylamine (DIPEA): the NIST (National Institute of Standards and Technology) value for proton affinity of DIPEA is 237.6 kcal/mol.

CONCLUSIONS

1. DIPEA/ICR provides unique opportunities for multidimensional analysis of complex sample matrices.
2. The Kendrick plots can be used to distinguish between different compounds in a sample.
3. Kendrick mass defect vs. Kendrick nominal mass provides additional dimensions for successful MS analysis.

REFERENCES