ACIDIC AND NEUTRAL POLAR NSO COMPOUNDS IN SMACKOVER OILS OF DIFFERENT THERMAL MATURITY REVEALED BY ELECTROSPRAY HIGH FIELD FOURIER TRANSFORM ION CYCLOTRON RESONANCE MASS SPECTROMETRY

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Introduction

Negative ion electrospray ionization (ESI) coupled with high field Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS) allows for the direct detection of acidic NSO compounds in petroleum. The technique requires no chromatographic separation, is able to distinguish 18 different compound classes (e.g., neutral nitrogen, carboxylic acids and oxygenates), and can identify ~14,000 distinct masses by ultra-high mass resolution and mass accuracy. We previously studied three crude oils from different geological origins [Organic Geochemistry 33 (2002b) 743–759]. Here, we expand our research by comparing two source-equivalent Smackover oils of different levels of thermal maturity. We observe clear differences in the distribution of NSO compound classes, types (number of rings plus double bonds within a class), and number of alkyl carbons. With increasing thermal stress, the relative amount of sulfur and oxygen containing compounds decreases, condensation and aromatization of the polar cores increase, and the number of alkyl carbons decreases, reflecting the distribution of saturated hydrocarbons.1

Results and Discussion

Figure 1 shows a mass scale-expanded segment of the spectrum of the negative ion ESI FT-ICR mass spectrum, for ions of nominal mass, 486 Da. Molecular formulas are abbreviated with their class and type (Z series that define the number of rings plus double bonds) designation. For example, -39 NS2 represents the homologous series CnH2n-39NS2. This molecule would contain 21 rings plus double bonds. Asterisks denote nuclides containing one (*) 13C atoms.

Figure 2 shows how polar molecules throughout the mass spectrum are distributed according to class (i.e., numbers of N, S, and O atoms in each elemental composition). Note the pronounced differences between the class distributions for Toxey and Turkey Creek oils. Toxey oil is a low gravity, high-sulfur crude, representing petroleum expelled from Smackover source rocks under relatively low maturity conditions, whereas Turkey Creek oil has appreciably higher gravity and lower sulfur, representing oil expelled from the Smackover source rocks under conditions associated with main-stage generation.

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References