Characterization of naphthenic acids in crude oils and naphthenates by electrospray ionization FT-ICR mass spectrometry

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We highlight the selective ionization of acidic components of crude oils and naphthenates by negative-ion electrospray ionization (ESI) Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS). Selective ionization by electrospray affords direct characterization of neutral nitrogen species and naphthenic acids in petroleum without derivatization or preconcentration of the sample, and with minimal sample consumption.

Angola and offshore Canadian crude oils and Athabasca bitumen were used as supplied. The sodium and calcium naphthenate deposits were collected from production separators and were used as supplied. Each sample was analyzed with a custom-built 9.4 T magnet (22 cm horizontal room temperature bore diameter) FT-ICR mass spectrometer at the National High Magnetic Field Laboratory in Tallahassee.

The ultrahigh resolution and mass accuracy of FT-ICR MS provide for detailed identification and compositional differences of acidic species in crude oils and naphthenates and also afford structural characterization of acids isolated from naphthenate deposits. Figure 1: Note that molecules with two oxygens (the primary component of naphthenates) have only one double bond (the C=O carbonyl), and thus are simply alkanoic acids (soaps).

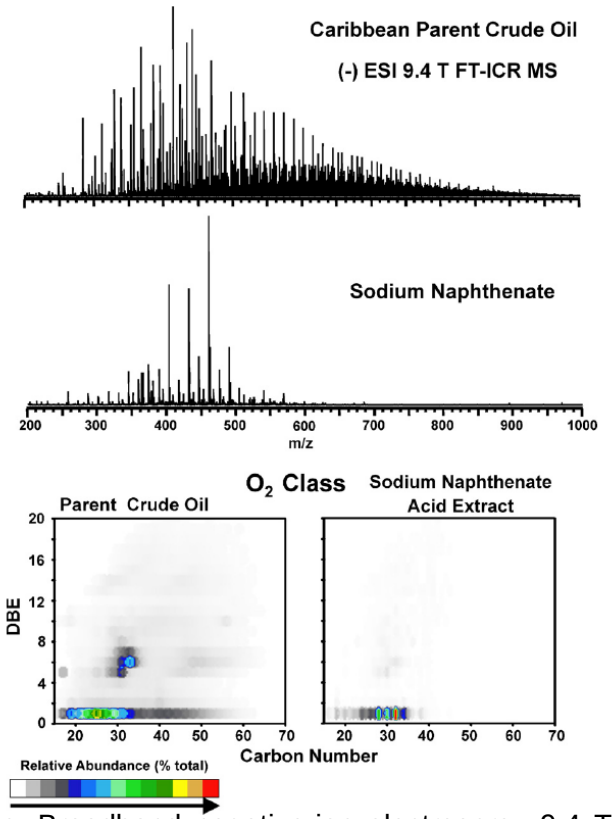

Fig. 1. Top: Broadband negative-ion electrospray 9.4 T FT-ICR mass spectra for a parent crude oil and acid extract from its associated sodium naphthenate emulsion or soap. Bottom: double bond equivalents (rings + double bonds) vs. carbon number images for O_2 class species from parent crude oil (left) and extract from sodium naphthenate (right).

Facilities: NHMFL 9.4 tesla widebore FT-ICR mass spectrometer.

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