Live

Petroleomics: Chemistry of the Underworld

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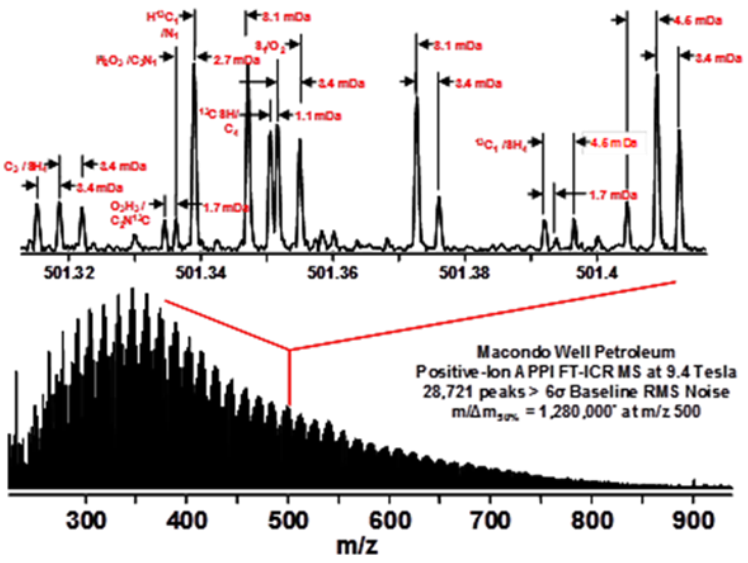
Abstract: Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) offers 10-100 times higher mass resolving power ($m/\Delta m_{50\%} > 1{,}000{,}000$ over a wide mass range) than any other mass analyzer, and is thus the mass analyzer of choice for complex mixture analysis. First, viewed only as a separation device, FT-ICR MS has 500x higher peak capacity than the best single-stage wet chemical separation (GC, LC, CE, gel, etc.). Thus, it becomes possible to separate complex mixtures *without* prior chromatographic or gel separation. Second, elemental composition may be determined from accurate (sub-ppm) mass measurement alone for unknown molecules up to ~1,200 Da. The chemical formula in turn reveals the numbers of N, O, and S (hetero) atoms (i.e., the compound "class"), the number of rings plus double bonds (DBE, or "type"), and the carbon number distribution (a measure of the degree of alkylation). We have resolved and assigned 125,000 peaks in a single petroleum 9.4 tesla FT-ICR mass spectrum, and even more at 21 tesla. Such vast data sets are best visualized from various graphical images scaled according to ion relative abundance: e.g., class distribution, Kendrick plot, van Krevelen plot, DBE vs. carbon number, etc.

Rapid advances in FT-ICR mass spectrometry have led a new field, Petroleomics, which aims to correlate and ultimately predict petroleum properties and behavior based on its detailed chemical composition. Applications include production deposit characterization, crude oil fingerprinting, crude oil compositional comparisons, heavy ends and asphaltene characterization, identification of naphthenic acids in crude oil and bitumen, biodegradation indices, emulsion stability, and polar compound speciation in the distillation process. The same principles apply to analysis of biofuels: e.g., 2nd generation (non-food crop sources) and 3rd generation (algae, whose body mass can contain up to 50% lipids).

In this talk, I shall review various technique developments and applications of FT-ICR MS, with particular attention to petroleum and its products (including the Macondo oil spill).



Tuesday Feb 14th, CB#204W at 11 am