Analysis of Complex Organic Mixtures by FT-ICR MS. Petroleomics

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Results and Discussion

Chromatographic techniques (primarily gas chromatography coupled with mass spectrometry (GC/MS) have been the most successful for environmental analysis. However GC/MS cannot cover the full compositional range inherent to very complex mixtures (e.g., petroleum) and is limited to volatile, low molecular weight compounds. This chapter reviews applications of Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) to analysis of complex mixtures of environmental importance: atmospheric contaminants, forensics (e.g., explosives), food products (e.g., wine, vegetable oils), role of microbes and plants in biodegradation of crude oil, abiotic weathering of oil spills, etc. For example, **Figure 1** shows the simultaneous resolution of molecules of elemental composition, CcHhOo, o = 1 to 18, according to number of oxygen atoms as well as the double bond equivalents (i.e., number of rings plus double bonds).[1]

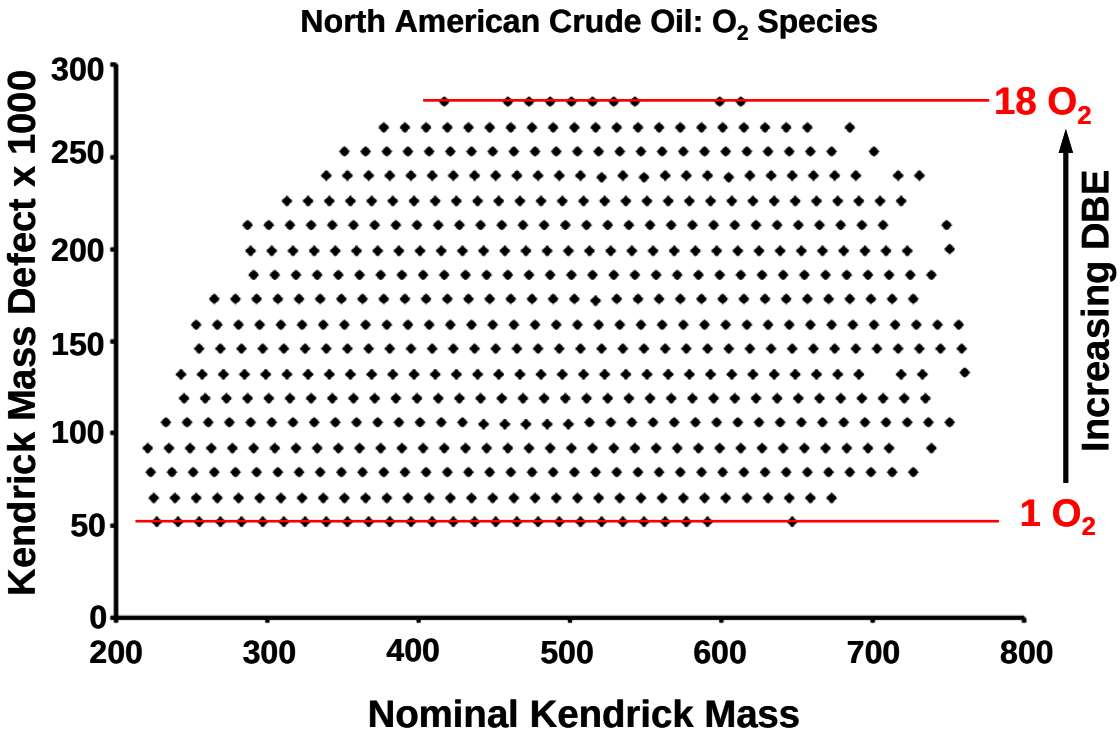

Figure 1. Plot of Kendrick mass defect (KMD) vs. nominal Kendrick mass for O_2 class species identified from the negative-ion ESI FT-ICR mass spectrum of a North American oil. Each increase in DBE displaces the data vertically, whereas each additional CH_2 group displaces the data horizontally. The use of Kendrick mass is explained elsewhere [2].

Acknowledgements

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References

[1] Lobodin, V. V., *et al.*, in *Comprehensive Environmental Mass Spectrometry*, Ed. A. Lebedev (ILM Publications, St. Albans, Hertfordshire, UK), ISBN 9781906799120, Chapter 18, pp. 415-442 (2012).
[2] Hughey, C. A., *et al.*, Anal. Chem., 73, 4676-4681 (2001).