Molecular Basis for Petroleum Distillation

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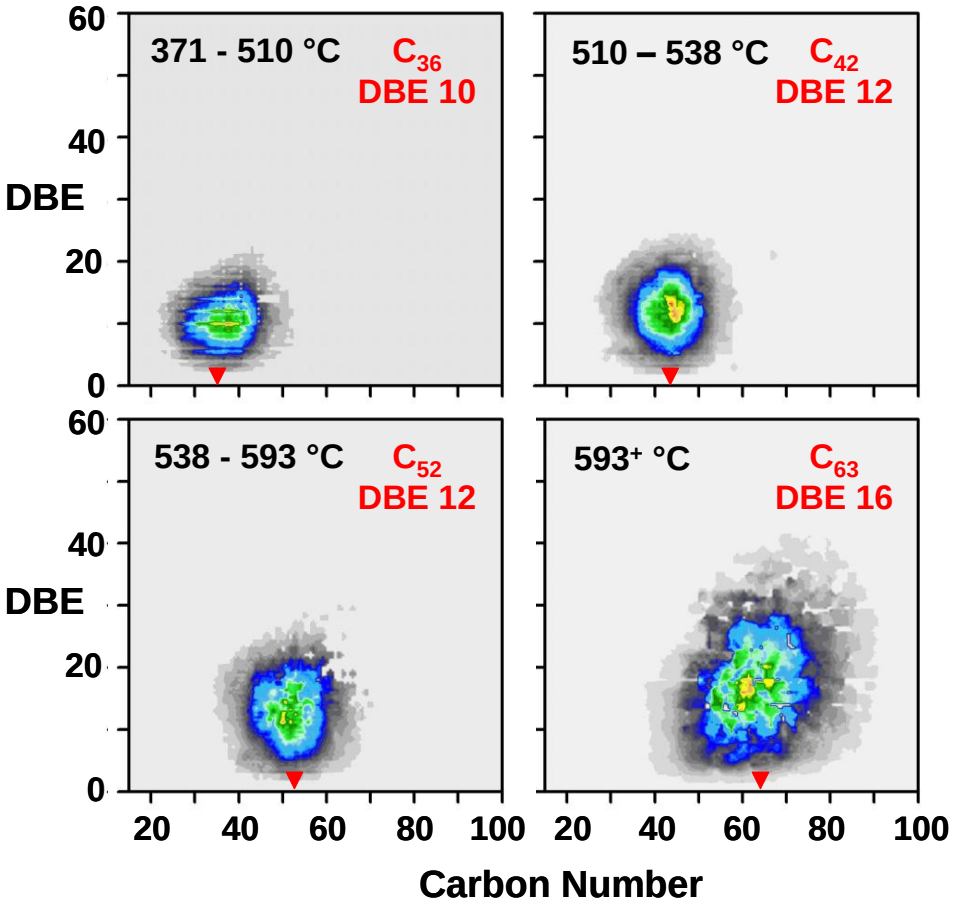
DMR-Award 0654118

Ion Cyclotron Resonance User Program

Petroleum crude oil refining produces various distillation products: naphtha, gasoline, jet fuel, kerosene, lube oil, etc. "Petroleomics", the complete and detailed chemical analysis of petroleum, has been enabled by applying the highest magnetic field to Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometry.

FT-ICR can sort the components of distillation products according to the number of Hydrogen, Carbon, Nitrogen, Oxygen and Sulfur atoms in each molecule. Or, as in the figure here, they can be sorted by the number of carbon atoms and "double bond equivalents (DBE = number of carbon rings plus double bonds). Note that the higher molecular weight components distill at higher temperature.



Number of molecules containing only carbon and hydrogen in a given petroleum distillation product, plotted versus number of carbon atoms and double bond equivalents (see text)

McKenna, A. M.; Purcell, J. M.; Rodgers, R. P.; Marshall, A. G. *Energy & Fuels* 2010, *24*, 2929-2938.

McKenna, A. M.; Blakney, G. T.; Xian, F.; Glaser, P. B.; Rodgers, R. P.; Marshall, A. G. *Energy & Fuels* 2010, *24*, 2939-2946.

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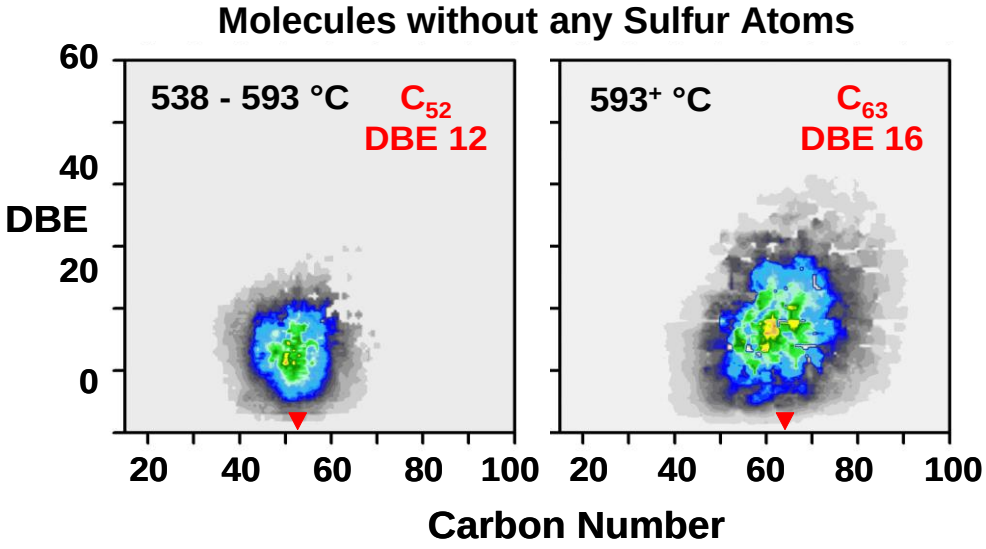

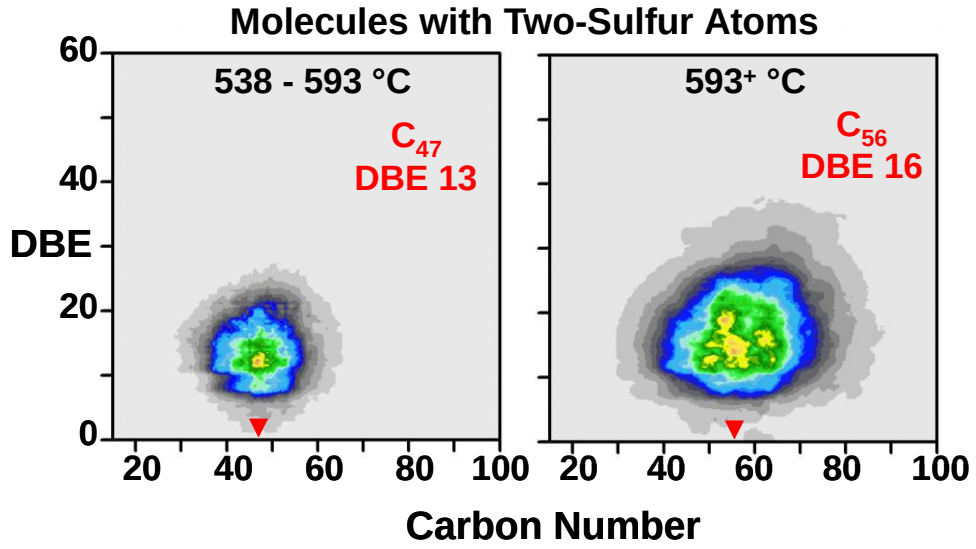

Petroleomics at high magnetic field reveals that the addition of each Nitrogen, Oxygen or Sulfur atom to a hydrocarbon molecule in petroleum requires removal of two or three carbons to produce the same boiling point: compare the red arrows for molecules with only carbon and hydrogen (top panels) to those for molecules with carbons, hydrogens and two sulfurs (bottom panels).

Thus, one can predict the (economically important) distillation profile for a crude oil, based on its detailed chemical composition--one of the first uses of "petroleomics" to predict the properties and behavior of crude oil. We are applying the same approach to predict deposits, corrosion, and formation of oil/water emulsions, and to monitor oil spills.