Advances in Asphaltene Petroleomics. Part 1: Asphaltenes Are Composed of Abundant Island and Archipelago Structural Motifs

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Introduction

The complex nature of asphaltenes creates inherent difficulties for FT-ICR MS analysis due to ionization efficiency differences between its components. Furthermore, the debate over the structure of asphaltenes, whether or not compounds are island (1 core) versus archipelago (multi-core) in nature, continues in the petroleum community. The work presented herein highlights a fractionation technique that both addresses the ionization differences for asphaltene components and separates them based on island and archipelago structure.

Results and Discussion

Asphaltenes were precipitated with *n*-pentane (C_5) and *n*-heptane (C_7), subsequently Soxhlet extracted with C_5 or C_7 to remove entrained maltenes; these are referred to as the purified asphaltenes. Purified C_5 asphaltenes were also Soxhlet extracted with C_7 to yield $C_{5\text{-}6}$ asphaltenes. This work shows that C_5 and $C_{5\text{-}6}$ asphaltenes ionize with the greatest efficiency and are comprised primarily of island-type structures, whereas the C_7 asphaltenes (50X lower ionization efficiency) are comprised primarily of archipelago-type structures; the correlation between ionization and structure indicates a link between structure and aggregation.

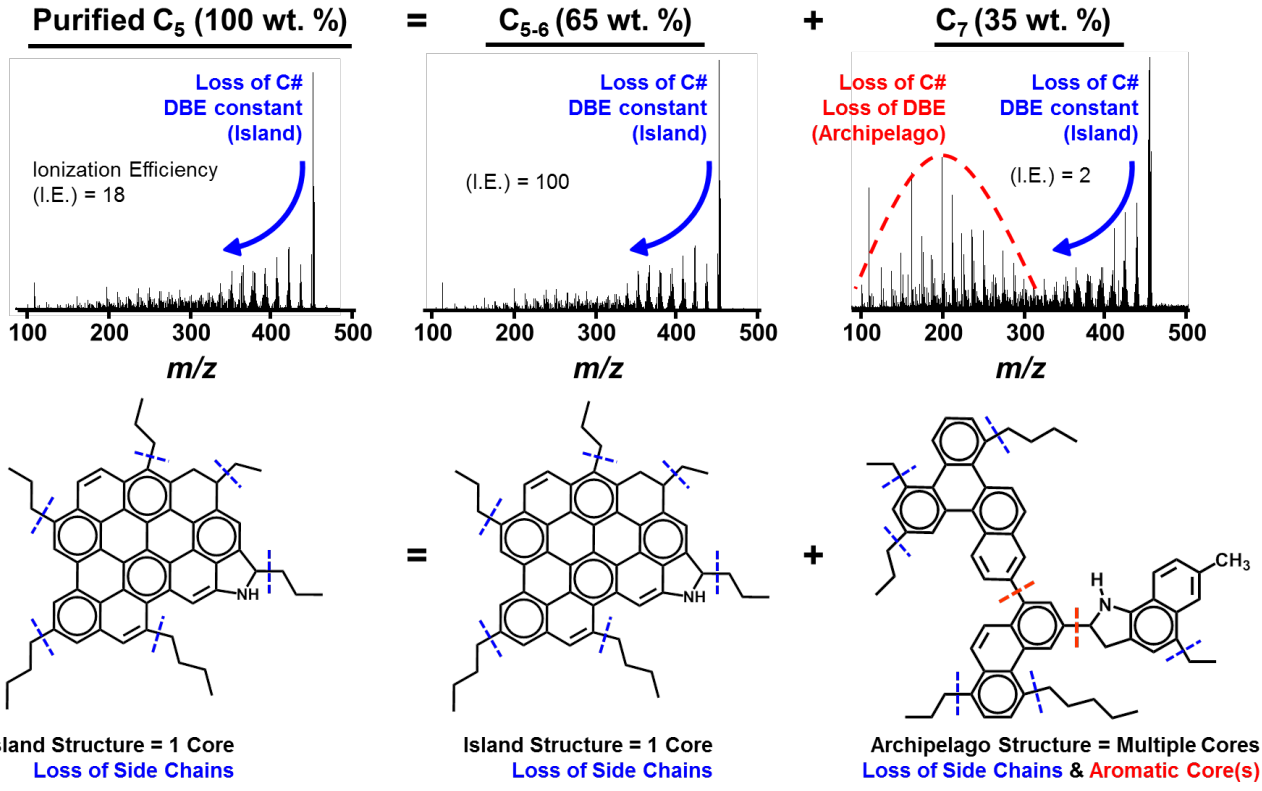

Fig. 1 shows the (top) fragmentation spectra for an isolated mass segment from C_5, $C_{5\text{-}6}$, and C_7 asphaltenes and (bottom) the representative structures for each type of fragmentation pathway. Island structures lose alkyl side chains (blue arrows (top), and blue dashed lines (bottom)) that reduce the carbon number, but not the aromaticity. Conversely, archipelago structures lose both carbon number and aromaticity (red dashed lines (top & bottom)) to yield a characteristic fragmentation pattern (top).

Acknowledgements

A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement #DMR-1157490 and the State of Florida. This work was also supported by FSU's Future Fuels Institute for access to instrumentation and financial support.

References

[1] Chacón-Patiño, M. L., *et al.*, Energy & Fuels, 31, 13509-13518 (2017).