Carbon fibers are essential for many applications, including aerospace and medical devices. Most fibers are made from polyacrylonitrile, which is quite expensive. Carbon fiber manufacturing from low-value petroleum feedstocks, which are highly enriched in asphaltenes, could decrease precursor costs by as much as 90%, and reduce greenhouse gas emissions. Asphaltenes are comprised of polycyclic aromatic hydrocarbons (PAH) organized into two structural motifs, as shown in Figure 1. “Single-core” PAH are fused into a single planar unit, whereas “multicore” compounds contain several smaller PAH units linked by flexible covalent bonds. Successful transformation of asphaltenes into carbon fibers requires a detailed understanding of how thermal treatment affects their composition and fiber stability. For example, sulfur-containing PAH (PASH) releases carbon disulfide bubbles within the fibers, diminishing fiber performance.

In this work, MagLab users investigated correlations between carbon fiber production processes and asphaltene composition. Asphaltene-enriched feedstocks were thermally treated under different conditions to direct their chemistry. Samples were characterized by 21T FT-ICR MS and gas-phase fragmentation (MS/MS spectra, Figure 1). The results indicate that severe thermal treatment yielded bad source material molecules (Figure 1 upper right), which in MS/MS revealed building blocks (blue arrow) consistent with single-core, high-molecular-weight PAH/PASH. No stable carbon fibers could be produced from these samples. Conversely, a feedstock treated with mild thermal conditions in molten sodium, a process designed to remove sulfur, yielded good source material molecules (Figure 1 lower right). Those compounds contained abundant multicore structural motifs, as shown by the abundant presence of low-molecular-weight PAH (yellow dashed line). These materials produced stable carbon fibers. Thus, the investigation of complex asphaltene composition by 21T FT-ICR MS with gas-phase fragmentation guides feedstock upgrading into effective carbon fiber precursors.

Facilities and instrumentation used: ICR User Facility, 21T FT-ICR Mass spectrometer
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