Title: Fragmentation-Resistant Polycyclic Aromatic Hydrocarbons (PAHs) for Investigating the Kinetics of Mesophase Formation

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Short abstract: Significant improvements to the methods used to produce advanced carbon materials from carbonaceous pitches have not occurred in years. While there are several processing technologies for synthesizing pitch-based carbon materials, the polydisperse nature of pitches has made the needed fundamental investigations into the kinetics of formation, along with the desired composition–property relationships, problematic. Thus, our team is using pure polycyclic aromatic hydrocarbons (PAHs) that undergo minimal fragmentation to investigate the fundamentals of pitch and mesophase synthesis. Pyrene is known to be a PAH that undergoes minimal fragmentation during oligomerization to a pitch, either in the presence or absence of a catalyst. Previous work indicates that pure pyrene trimer forms a discotic nematic mesophase at temperatures under 300 °C, so optimization of the lower molecular weight (MW) “mers” in the resultant pitches is of interest. Kinetic investigations at 200-400 °C in the presence of $AlCl_3$ catalyst indicate that as much as 50% of the feed can be converted to dimers and trimers with proper control of the reactor time and temperature. Another PAH of significant practical interest is naphthalene. The pioneering work of Mochida et al. with naphthalene-based mesophase pitches showed us that extensive fragmentation occurs in the presence of HF/BF_3 catalyst; however, our recent work indicates that higher-temperature oligomerization without catalyst results in surprisingly clean mass spectra consisting of just a few oligomers. Identification of mesogenic species and maximizing the concentration of such species in a “clean” naphthalene pitch are goals of this work.