Probing Conjugation-Related Properties in Benzo- and Thieno-fused Dehydroannulenes

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Over the last 15 years, synthetic investigations of annulenes have experienced a vigorous resurgence. Much of the renewed interest can be attributed to the recognition that these compounds can potentially serve as precursors for a variety of technologically important, carbon-rich molecular and polymeric systems, such as novel allotropes of carbon, molecular scaffolds, and nonlinear optical materials. To systematically study the reaction chemistry and possible materials properties, researchers need easy access to differing DBA topologies on greater than milligram scale. We have developed synthetic methods that permit facile preparation of annulenes of virtually any shape, size, or substitution pattern. With the synthetic hurdles cleared, our aim is to construct novel annulene geometries and related structures, and to investigate of the chemical reactivity and physical properties of the macrocycles to answer fundamental scientific questions. Notable outcomes from these studies to date include:

- evidence of the global electronic delocalization within the hybrid macrocycles
- evidence that fusion of annulenes to cyclophanes weakens the aromaticity of the other moiety
- evidence that planarization of the macrocycles significantly enhances the electron delocalization