Negatively Curved Molecular Nanocarbons Containing Multiple Heptagons Are Enabled by the Scholl Reactions of Macrocyclic Precursors
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Introduction

Embedding heptagons in polycyclic aromatic frameworks gives rise to negatively curved molecular nanocarbons, which are not only key fragments of long-sought-after carbon schwarzites but also bring new opportunities to explore unprecedented nanocarbons with interesting properties. This study demonstrates the Scholl reactions of macrocyclic precursors as a general strategy for synthesizing negatively curved molecular nanocarbons containing different numbers of heptagons. The π-backbones containing multiple heptagons are significantly curved and rigid as revealed by density functional theory calculations and X-ray crystallography.

Synthesis

Suzuki-Miyaura Coupling

Yamamoto Coupling

Scholl reaction

Crystal Structures

Conformational Flexibility

Figure 1. (a)-(b) Calculated pathway for inversion of 1 and 6; All of the structures were calculated at the B3LYP/6-31G(d) level of DFT

Organic Field Effect Transistors

Figure 3. Drain current ($I_{DS}$) versus gate voltage ($V_{GS}$) with drain voltage ($V_{DS}$) at –35 V for a typical OFET of 3 on the CDPA/AlOx/SiO2 as measured in air with an active channel of W = 975 μm and L = 195 μm.

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References: